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ENFOR Project C-197(2)

Technical Assessment of Down Draft Wood Gasifiers

by

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February 1984

ABSTRACT

A mechanistic model has been developed for down-draft wood gasifiers. Each region of the gasifier is modelled, including drying, pyrolysis, combustion and gasification. A post-reaction region is included in the model for those locations in the gasifier where there is no reaction but simply a heating or cooling of the solid or gas. The model is one-dimensional - radial profiles are not considered. Axial profiles are predicted for composition (solid, water, hydrogen, methane, carbon monoxide, carbon dioxide, oxygen and nitrogen) and temperature.

The details of this model have been incorporated in a computer simulation package called QUGAS2. Modelling of the drying and pyrolysis zones gives reasonable results based on a comparison of predicted temperatures with data available in the literature. However, the results for the combustion and gasification zones are inconsistent with reported observations. A number of attempts have been made to determine whether the problem lies in the assumptions used in the model or in the mathematical solution techniques employed, but the question is still unresolved. This work is continuing.

Operating data produced by Saskatchewan Power Corporation using a down-draft imbert gasifier were analyzed. In addition to using these data for comparison with the mechanistic model, an empirical model was formulated. Gas production rate, gas temperature, maximum gasifier temperature, higher heating value of the gas and the carbon monoxide to hydrogen ratio of the gas were regressed as functions of the wood particle size, the wood moisture content, the electrical load on the gasifier (proportional to the air feedrate), the preheated air temperature, and the

grate agitation rate.

Finally, the problems associated with collecting reliable gasifier operating data were examined. Techniques for obtaining and analyzing gasifier data are suggested.

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1. INTRODUCTION

In the last decade, rising oil prices have spurred interest in the development of alternate energy sources. As part of Canada's response the ENFOR research program was established to assess the utility of the forests as one alternative energy source. This project is part of the ENFOR program.

Forest products, notably wood and biomass, are bulky and nonhomogeneous and are thus difficult to transport and process. Fortunately, one relatively simple method exists for processing wood and biomass - gasification. In gasification, the solid fuel is converted to a gaseous fuel, and this gaseous fuel can be used in a wide variety of applications because it is easily stored, and combusted.

However, the gasification of wood is complicated by the production of tars which can ruin processing equipment. The evolution of gasifier designs has revealed that some configurations yield significantly lower amounts of tars, the best design for this purpose being the down-draft wood gasifier.

In this project, ENFOR Contract C-197, the down-draft wood gasifier has been examined in detail. The major objectives were to develop and test quantitative methods to assess the operation and design of down-draft wood gasifiers, including:

i) mechanistic and empirical models of down-draft wood gasifiers

ii) computer simulation programs incorporating these models

iii) experimental design and data analysis procedures to obtain data, and extract information efficiently, for assessing and improving the operation of down-draft wood gasifiers

iv) procedures for establishing limits on the reliability and acceptability of data from gasifier operation.

2. THE MECHANISTIC MODEL

Many mechanistic models of gasification appear in the literature. Yoon et al [1] have developed a model of an up-draft coal gasifier, Desrosier and Richey [2] have developed a model of an up-draft wood gasifier, and Tabatabaie-Raissi [3] and Groeneveld [4] have developed models of down-draft wood gasifiers. Groeneveld's model is applicable to the gasifier design which is modelled in this project. However, he has focussed attention on the gasification reactions alone. Drying, pyrolysis and combustion are treated as a single black box process, with the gaseous products of this black box being carbon dioxide and steam resulting from combustion of the gaseous pyrolysis products. The up-draft gasifiers modelled by Yoon et al and by Desrosiers and Richey are significantly different in their operational behaviour and therefore these models are not directly applicable to the down-draft wood gasifier.

In this project, the down-draft wood gasifier is modelled, with attention being given to the application of mechanistic theory for each of the drying, pyrolysis, combustion and gasification reactions.

However, despite the above differences, much of the mechanistic theory is common to all gasifier models. Comparison of the model developed in this project with those models mentioned above will make this obvious.

At the top of a down-draft gasifier, such as the Imbert gasifier shown in Figure 1, the wood is wet and the gas in the void space surrounding each wood particle is simply moist air. As the wood moves down through the bed, the temperature rises and the wood dries and devolatilizes to leave a solid char. At an intermediate point along the

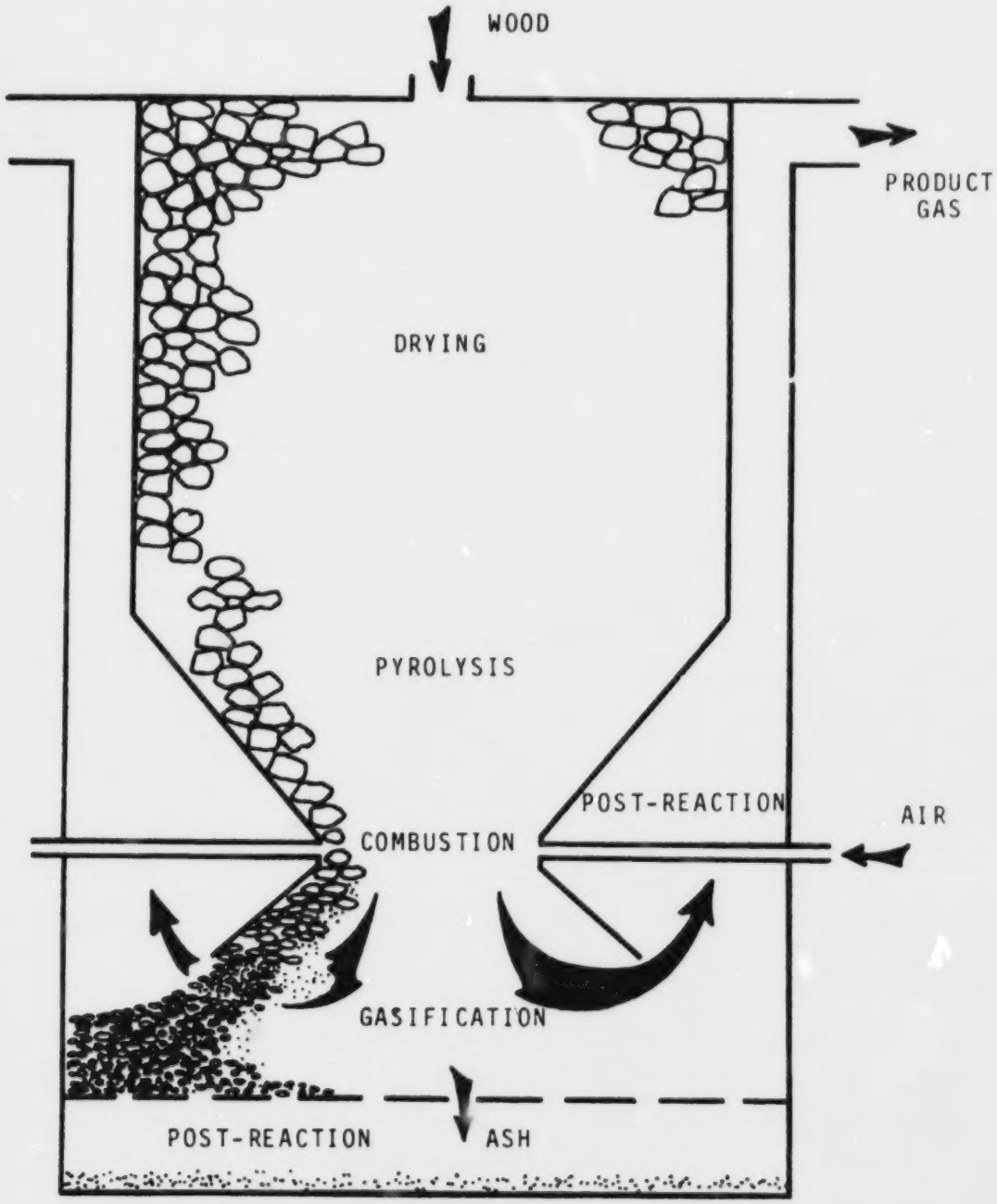

Figure 1 : The Imbert Down Draft Gasifier

length of the gasifier, air is injected and, in the vicinity of this blast, the char and gases combust. Further down in the bed, the char is gasified until it is completely converted to ash, or until it is removed from the gasifier, or until the temperature falls below 750°C.

In actual operation it is suspected that the above reactions occur in overlapping regions, with pyrolysis commencing before drying is complete, combustion commencing before pyrolysis is complete, etc. However, in this modelling effort the reaction zones have been considered to be separate. The progress of wood conversion is divided into five separate reaction zones: drying, pyrolysis, combustion, gasification and post-reaction.

Although the basic mechanistic theory which is incorporated into this model is expected to be applicable in the evaluation of many different designs of down-draft gasifiers, the current form of the model is set up to simulate the operation of an Imbert-type gasifier. In the Imbert design, the moving packed bed is surrounded by an annulus through which the product gases flow before exiting from the gasifier.

Solid and gas are assumed to move down through the bed in plug flow, and therefore only axial profiles of composition are generated. However, heat transfer occurs radially as well as axially. This radial transfer implies the existence of a radial temperature gradient, which in turn implies a radial concentration gradient. This complication in modelling the gasifier is removed by the simplifying assumption that there are three radial zones, viz. the bed, the annulus, and the environment, which are at uniform but different temperatures. This involves the assumption that the resistances to radial heat transfer are concentrated at the walls between these radial zones.

The heat and mass fluxes in each of the zones of the gasifier are characterized by ten ordinary differential equations. Nine of these equations are first order and trace the conversion of solid and production of gaseous products (Tables 1 and 2) in terms of individual component flowrates. Water, hydrogen, methane, carbon monoxide, carbon dioxide, oxygen and nitrogen are the only gaseous species which are considered to be present in the gasifier. Wood, char and ash are the only solid species and tar production is not considered. These assumptions are supported by experimental results in the literature. The tenth equation, representing the energy balance, is second order and traces the change in temperature with axial position in the gasifier.

For numerical solution, the gasifier is divided into the five reaction zones. At a number of intermediate points within each of these zones, the physical properties,gasifier dimensions and heat transfer coefficients are updated to account for the computed local position, temperature and composition. The ten differential equations are solved simultaneously.

Transfer from one reaction zone to the next is controlled by the following zone boundary conditions:

Table 1 : Independent Variable Nomenclature

Variable	Reference
solid carbon mass flowrate	F_C
gaseous water mass flowrate	F_{H_2O}
hydrogen mass flowrate	F_{H_2}
methane mass flowrate	F_{CH_4}
carbon monoxide mass flowrate	F_{CO}
carbon dioxide mass flowrate	F_{CO_2}
oxygen mass flowrate	F_{O_2}
nitrogen mass flowrate	F_{N_2}
solid mass flowrate	F_s
temperature	T
dT/dz	dT/dz (or U)

F_i is in kg s^{-1}, T in K and z in m.

Table 2 : Chemical Reactions Occurring in the Gasifier

Reaction	Reference Name	#
wet wood (H_2O (L)) $\longrightarrow$ dry wood (H_2O (G))	Drying	1
dry wood $\longrightarrow$ char + gases	Pyrolysis	2
$H_2 + 1/2\ O_2 \longrightarrow H_2O$	Homogeneous Comb.	3a
$CH_4 + 2\ O_2 \longrightarrow CO_2 + 2\ H_2O$	Homogeneous Comb.	3b
$CO + 1/2\ O_2 \longrightarrow CO_2$	Homogeneous Comb.	3c
$\lambda C + O_2 \longrightarrow 2(\lambda-1)CO + (2-\lambda)CO_2$	Combustion	3d
$C + H_2O \longrightarrow CO + H_2$	Gasification	4
$C + CO_2 \longrightarrow 2\ CO$	Gasification	5
$C + 2\ H_2 \longrightarrow CH_4$	Gasification	6
$CO + H_2O \longrightarrow CO_2 + H_2$	Water-Gas Shift	7

i) THE DRYING-PYROLYSIS BOUNDARY

Drying is considered to be complete when all of the water in the wood has been evaporated. The amount of water in the wood is determined from the recorded moisture content (wt% dry basis) of the wood feedstock.

ii) THE PYROLYSIS-COMBUSTION BOUNDARY

The combustion zone is considered to commence at a position in the gasifier which is a "half-width" above the centre-line of the air injection tuyeres. The "half-width" measurement is an adjustable parameter in this model representing the extent of the air dispersion. (In the vicinity of the tuyeres, the air injected via the tuyeres is superimposed on the downward gas flow from the pyrolysis region according to an air distribution model which is partially defined by this "half-width measurement.) However, both SERI [2] and Groeneveld [4] report that this "half-width" dimension is limited to a few particle diameters. In their studies this corresponded to a few centimetres.

iii) THE COMBUSTION-GASIFICATION BOUNDARY

The combustion zone is considered to be complete when all of the oxygen has been consumed. This occurs somewhere beyond a "half-width" below the centre-line of the tuyeres.

iv) THE GASIFICATION-POST REACTION BOUNDARY

Three criteria apply here. The boundary between these zones is reached when any one of the following conditions occurs: i) the char is completely consumed or ii) the grate level is reached or iii) the temperature drops below 750 °C.

2.1 Drying

At the top of the down-draft gasifier, where movement of both the solid and gas phases is very slow and the temperature is low, the wood dries.

$$H_2O\ (L) \longrightarrow H_2O\ (G) \qquad \text{(Reaction 1)}$$

Due to the relatively long gas-solid contact times the gas becomes saturated with water vapour at the local temperature in the bed. The rate of drying is then determined solely by the flux of heat to this zone through the walls from the annulus and from lower regions of the bed.

2.1.1 Mass and Energy Balances for the Drying Zone

The differential equations which govern behaviour in the drying zone are:

$$\frac{dF_{H_2O}}{dz} = \frac{(F_{N_2} + F_{O_2})}{M_{air}} \frac{M_{H_2O}}{P} \frac{dP^{sat}_{H_2O}(T)}{dz}$$

$$\frac{dF_s}{dz} = - \frac{dF_{H_2O}}{dz}$$

$$\frac{dF_i}{dz} = 0 \qquad \text{for } i = C,\ H_2,\ CH_4,\ CO,\ CO_2,\ O_2,\ N_2$$

where

$$\frac{d(P^{sat}_{H_2O}(T))}{dz} = \left[\frac{d(P^{sat}_{H_2O}(T))}{dT} \right] \left[\frac{dT}{dz} \right]$$

Keenan et al [5] have reported the following expression for the saturated vapour pressure of water as a function of temperature:

$$\frac{p^{sat}_{H_2O}}{p^{crit}} = \exp\left[\tau \times 10^{-5}(T^{crit}-T)\sum_{I=1}^{8} B_I(0.65-0.01T)^{I-1}\right]$$

where $p^{sat}_{H_2O}$ is the saturated vapour pressure (atm)

p^{crit} is the critical pressure (217.99 atm of water)

$\tau = 1000/T$ (T in K)

T^{crit} is the critical temperature (374.136 °C)

T is the temperature (°C)

$B_1 = -741.9242$ $\quad B_5 = 0.1094098$
$B_2 = -29.72100$ $\quad B_6 = 0.439993$
$B_3 = 11.55286$ $\quad B_7 = 0.2520658$
$B_4 = 0.8685635$ $\quad B_8 = 0.005218684$

F_I is the axial mass flowrate (kg/s) of component I, and z is the axial position in the gasifier, measured from the top of the bed.

The energy balance is derived according to the method described in Section 2.6.

$$\frac{d^2T}{dz^2} = \frac{(\Sigma(F_I C_{pI}) + \Delta H_1 \frac{(F_{N_2}+F_{O_2})}{M_{air}} \frac{M_{H_2O}}{P} \frac{d\,p^{sat}_{H_2O}}{dT}) \frac{dT}{dz} - 2\pi r h_w (T_a - T)}{k_e A'}$$

where T_a is the temperature in the annulus at the same axial position z.

F_{N_2}, F_{O_2} and terms relating to "air" account for dilution of the gas phase by air which is held up in the void spaces between the wood particles during feeding. In this model it is assumed that the total pressure in the suction down-draft gasifier, P, doesn't exceeds one atmosphere.

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$$\frac{d^2T}{dz^2} = \frac{\left(\Sigma(F_i C_{pi}) + \Delta H_1 \frac{(F_{N_2}+F_{O_2})}{M_{air}} \frac{M_{H_2O}}{P} \frac{d\,p^{sat}_{H_2O}}{dT}\right)\frac{dT}{dz} - 2\pi r h_w(T_a-T)}{k_e A'}$$

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2.2 Pyrolysis

Pyrolysis, or devolatilization, is a complex thermal decomposition of solids. It has not been given much attention in previous work on the modelling of gasifiers, largely due to the complexity of the reaction. Anthony and Howard [6] have produced a comprehensive review of the extensive information available on the pyrolysis of coal, however there is no similar document available for the literature on the pyrolysis of wood.

The pyrolysis of wood is reported to be affected by a number of factors: the heating rate of the solid, the final temperature attained during the decomposition, the size of the solid particle being pyrolyzed, the composition and pressure of the atmosphere in which the decomposition occurs and the catalytic properties of the ash which is associated with the solid. To date, reports of the effects of these factors are largely qualitative.

As a result of the complexity of the pyrolytic process and the uncertainties associated with it, a simplified model of pyrolysis has been developed which combines decomposition kinetics with a product distribution.

2.2.1 The Product Distribution

The products of pyrolysis include carbon dioxide, carbon monoxide, hydrogen, methane, water, char and tar. However, since the character and production of pyrolytic tars is poorly understood tar production is ignored in this model. Fortunately, tar production is insignificant in the down-draft gasifier and this omission will have little effect on the validity of the model predictions.

The char is assumed to be a pure carbon solid. This assumption facilitates modelling of the solid reaction behaviour in subsequent reaction zones. In this model the char yield is the fixed carbon yield estimated from the proximate analysis of the wood. It should be noted, however, that the procedures used for determining the proximate analysis were originally developed for coal, not for wood.

The pyrolytic gases are modelled separately. On a wet basis,

$$X_{H_2O} + X_{H_2} + X_{CH_4} + X_{CO} + X_{CO_2} = 1 \qquad (1)$$

where X_i is the mol fraction of gaseous species i evolved during pyrolysis.

However, production of the pyrolytic gases is usually reported on a dry gas basis. Maa [7], Brink and Massoudi [8], Simmons and Sanchez [9] and Deglise [10] have each reported this type of gaseous product distribution (Figure 2). In general, these studies reveal similar behaviour of the distributions as a function of temperature:

I) Carbon dioxide yield falls off rapidly as temperature increases [7,8,9,10].

II) Methane production is approximately constant above 600°C [7,8,9,10], at a value of

$$\frac{X_{CH_4}}{X_{H_2} + X_{CH_4} + X_{CO} + X_{CO_2}} = 0.15 \qquad (2)$$

III) Carbon monoxide and carbon dioxide yields cross

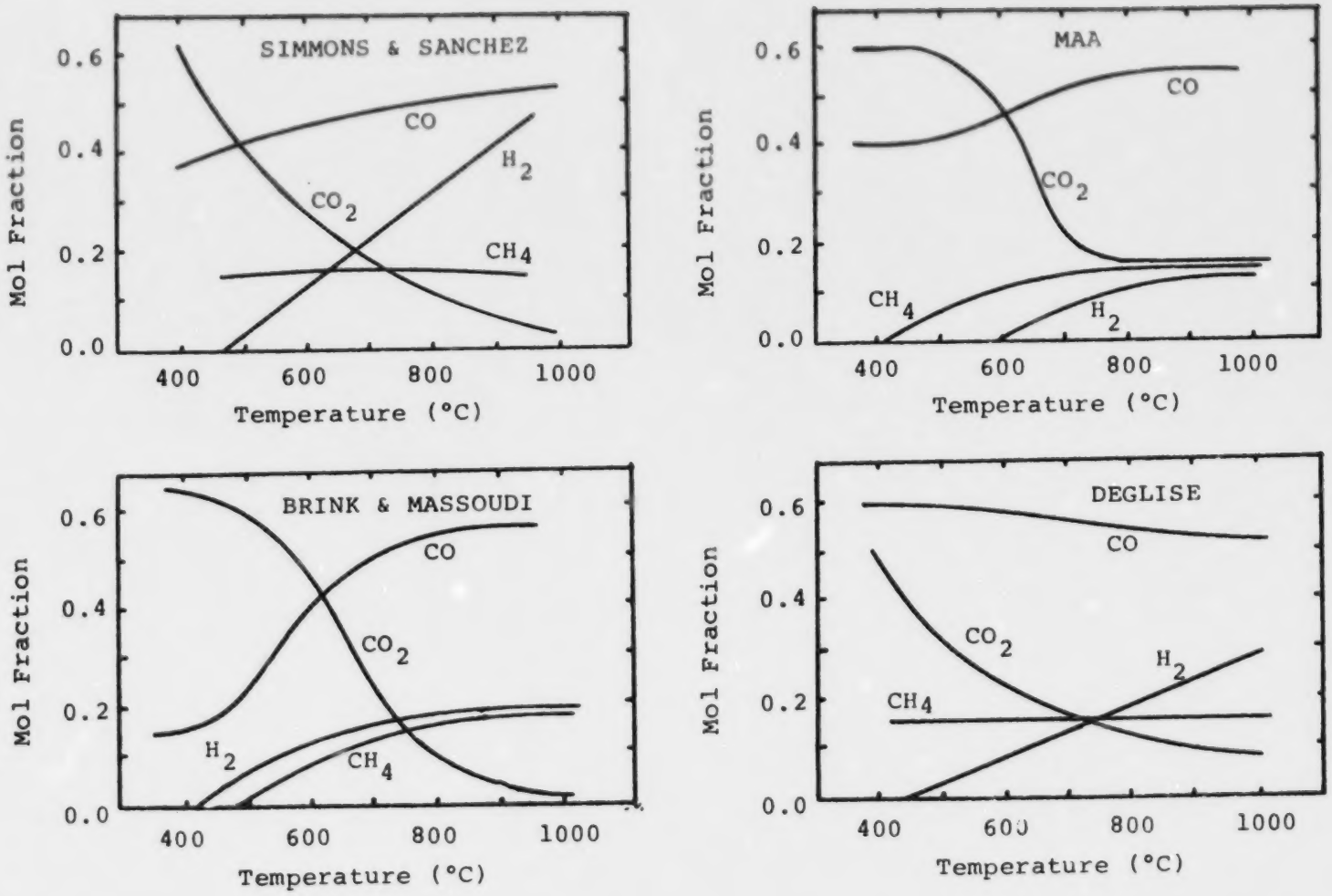

Figure 2 : Pyrolytic Gas Distributions (dry gas basis)

over in the temperature range 300 - 750°C [7,8,9].

Methane and carbon dioxide yields also cross over in the temperature range 300-750°C [8,9,10].

iv) The carbon monoxide yield increases with temperature [7,8,9].

The wood particle is assumed to pyrolyze in an unreacted shrinking core manner, where decomposition occurs at a sharply defined reaction interface. In the shrinking core model all solid between the interface and the centre of the particle is virgin solid (in this case wood) and all solid between the interface and the surface of the particle is completely reacted (in this case a pure carbon char and ash). Therefore, the full complement of pyrolytic products (including char) evolved at any time and temperature must have an overall carbon/hydrogen/oxygen composition the same as that of the virgin wood. The following constraints result:

$$\frac{X_{CH_4} + X_{CO} + X_{CO_2}}{X_{H_2O} + X_{CO} + 2X_{CO_2}} = \frac{X_C^P}{X_O^P} \qquad (3)$$

$$\frac{X_{H_2O} + X_{CO} + 2\,X_{CO_2}}{2X_{H_2O} + 2X_{H_2} + 4X_{CH_4}} = \frac{X_O^P}{X_H^P} \qquad (4)$$

where X_j^P is the atomic fraction of element j in the volatile fraction of the wood (dry basis) (determined from the proximate and ultimate analyses of the wood - see Appendix A.1.1)

One further constraint is necessary to characterize the product distribution fully. The constraint which was

finally selected is

$$\frac{X_{CH_4}}{X_{CO_2}} = R_h \qquad (5)$$

where R_h = 0.7, 0.85, 1.0, 1.15, 1.30
at 400, 500, 600, 700 and 800 °C, respectively
as determined by an averaging of the behaviour
of the four cited distributions.

Using constraints 1 to 5 above a complete pyrolytic product distribution is described (Figure 3). The high hydrogen yield is a result of the assumption of a pure carbon char - the elemental hydrogen associated with the actual solid hydrocarbon which is produced appears as an increase in the gaseous hydrogen yield. Despite the high hydrogen yield, this formulated product distribution still shows the four common characteristics of the original gaseous distributions (i - iv) mentioned above.

2.2.2 The Kinetics of Pyrolysis

Tran [11] has reported a kinetic model for the pyrolysis of wood which is a function of solid conversion and temperature.

$$-\frac{1}{W_o}\frac{dW}{dt} = k_2 \frac{W}{W_o} \exp(-E_2/RT)$$

where $E_2 = E_2^o + aX$

$$X = \frac{W_o - W}{W_o}$$

W_o, W are the initial mass of the wood and the mass of solid remaining at time t, respectively

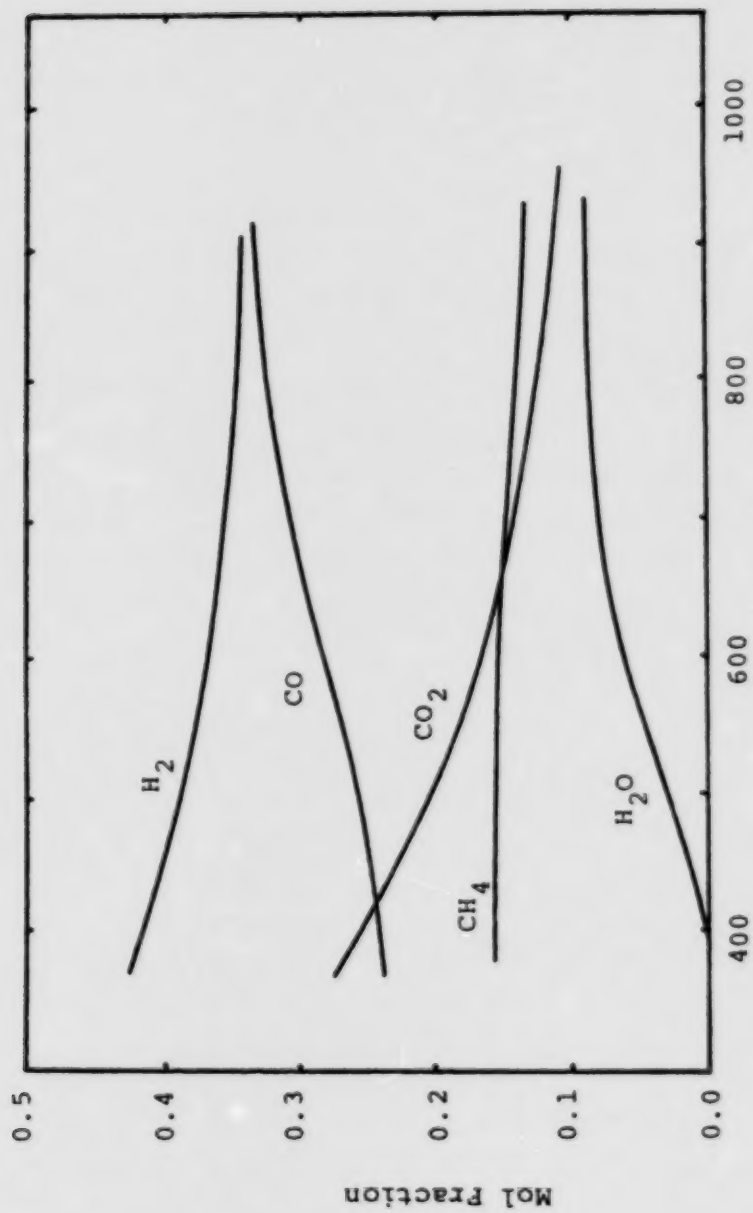

Figure 3 : Final Pyrolysis Product Distribution

$$22 < a < 35 \quad \text{(kcal/mol)}$$

$$1.6\times10^{9} < k_2 < 1.6\times10^{10} \quad (\text{min}^{-1})$$

$$21 < E^{\circ}_2 < 27 \quad \text{(kcal/mol)}$$

Rearranging to a form appropriate for use in this gasifier model, the expression for the rate of pyrolysis becomes

$$R_2 = \frac{k_2}{60} \rho_{bed}(1-X) \exp(-E_2/RT) \qquad (\text{kg s}^{-1}\text{m}^{-3})$$

The predictions of this kinetic model are consistent with the results of Mackay and Roberts [12] who report that 50% to 80% of the solid weight loss is complete below 500°C (773 K) (Figure 4).

2.2.3 The Thermodynamics of Pyrolysis

The heat of pyrolysis has been reported to be exothermic, endothermic and thermally neutral by different researchers. This disagreement is probably due to different experimental conditions such as heating rate, maximum temperature, etc., as is the variety of reported product distributions.

In the face of these inconsistencies, the heat of pyrolysis is calculated from a thermodynamic basis using the selected pyrolysis product distribution. This approach has shown that the heat of pyrolysis can vary from slightly exothermic to slightly endothermic, depending on the nature of the product distribution.

In this model, the heat of pyrolysis is computed as the difference between the enthalpy of combustion of dry wood and the enthalpy of combustion of the pyrolysis products

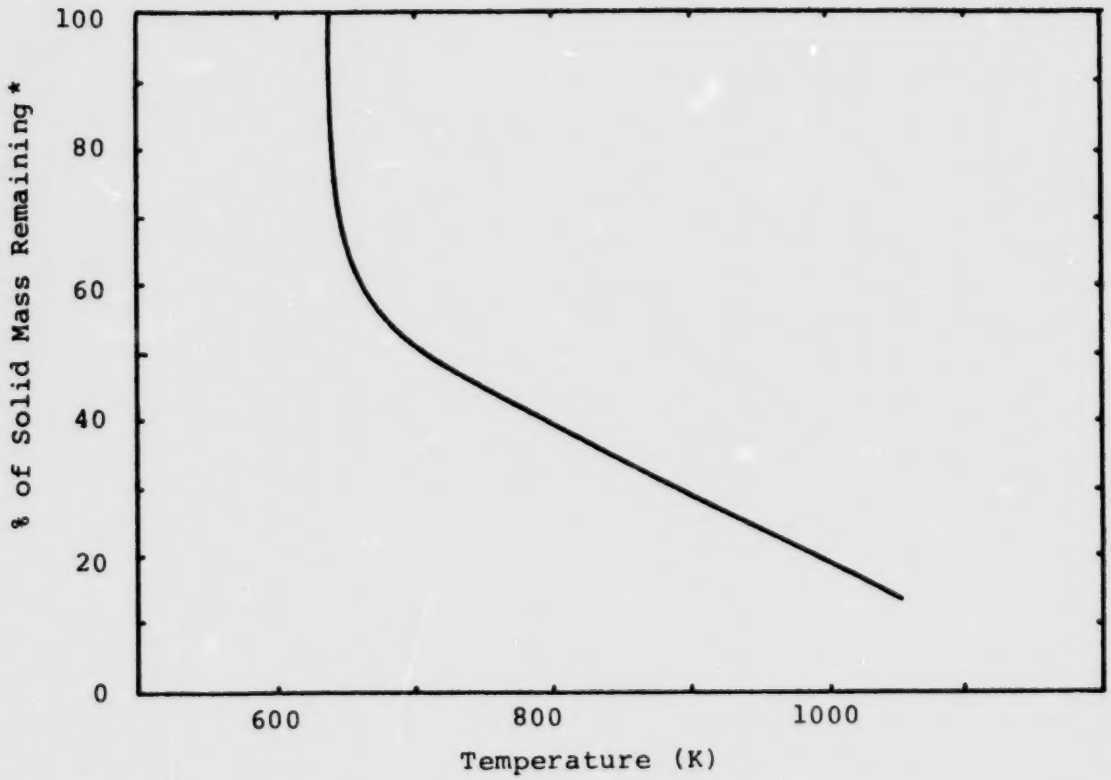

Figure 4 : Mass Loss During Pyrolysis

* 100 % represents the initial mass of dry wood.

(Figure 5).

$$\Delta H^{pyr}_{wood,298K} = \Delta H^{comb}_{wood,298K} - \Delta H^{comb}_{pyr\ product,298K}$$

The IGT equation [13] is used to compute the enthalpy of dry wood combustion:

$$\Delta H^{comb}_{wood,298K} = -232.6\ [146.58C + 568.78H + 29.45 - 6.58A - 51.53(O+N)]$$

where ΔH (kJ/kg dry wood)
C,H,A,O,N represent the elemental carbon, hydrogen ash, oxygen and nitrogen (wt % dry basis) in the wood (from the ultimate analysis)

Enthalpies of combustion for the pyrolytic products (Table 3) are obtained from Smith and Van Ness [14].

Using this technique and the pyrolytic product distribution developed in Section 2.2.1 the computed heat of pyrolysis ranges from 200 to 500 kJ/kg of dry wood, indicating that the decomposition is slightly endothermic under these conditions. Compared to the enthalpy of combustion of wood, -19500 kJ/kg of dry wood, this value is very small. This prediction produces results which are not significantly different from those generated when the heat of pyrolysis is assumed to be zero (thermally neutral).

2.2.4 Mass and Energy Balances for the Pyrolysis Zone

The differential equations which govern the pyrolysis zone combine the product distribution, decomposition kinetics and thermodynamics developed above. These equations are:

$$\frac{dF_s}{dz} = -R_2 A'$$

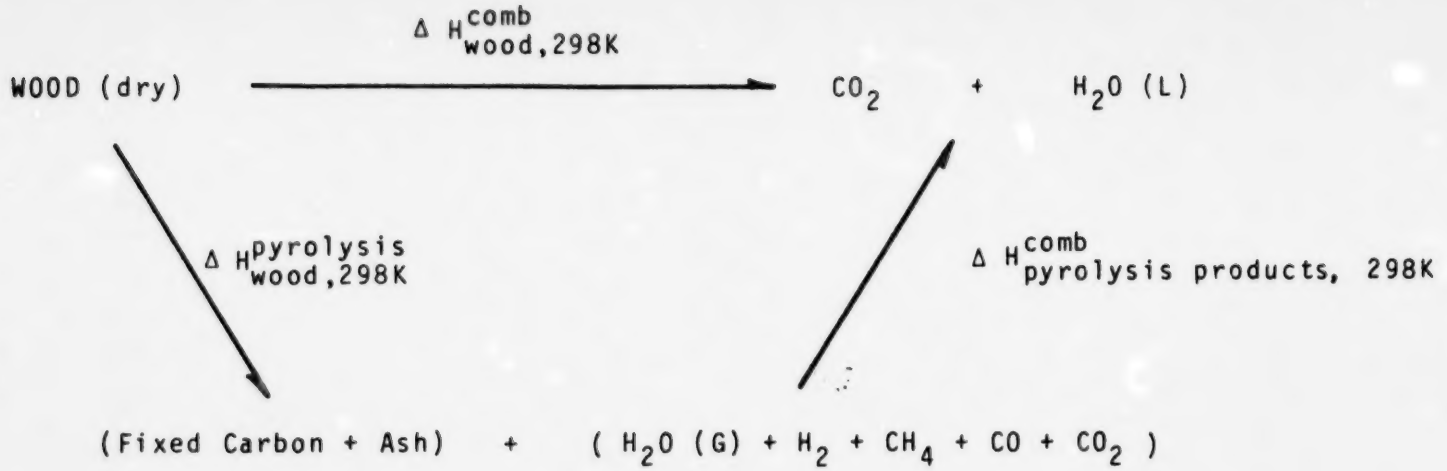
Δ H comb wood,298K
WOOD (dry)
CO2 + H2O (L)
Δ H pyrolysis wood,298K
Δ H comb pyrolysis products, 298K
(Fixed Carbon + Ash) + (H2O (G) + H2 + CH4 + CO + CO2)

Figure 5 : Calculation of the Heat of Pyrolysis

Table 3: Standard Enthalpies of Combustion [14]

Species	ΔH_{298K}^{comb} (kJ/kg)
C	-3.279×10^4
H_2	-1.429×10^5
CH_4	-5.565×10^4
CO	-1.011×10^4
CO_2	0.0

The products of combustion are $H_2O(L)$ and CO_2.
For $H_2O\ (G) \longrightarrow H_2O(L)$, $\Delta H^{cond} = -2.445 \times 10^3$ (kJ/kg).

$$\frac{dF_i}{dz} = R_2 A' e_i \qquad \text{for } i = H_2O,\ H_2,\ CH_4,\ CO,\ CO_2$$

$$\frac{dF_i}{dz} = 0 \qquad \text{for } i = O_2,\ N_2,\ C$$

where R_2 is the apparent rate of pyrolysis (developed in Section 2.2.2)

A' is the cross-sectional area of the gasifier

e_i is the mass fraction of species i evolved during pyrolysis (see the product distribution in Section 2.2.1)

In the pyrolysis zone the solid, whether wood or char, is attributed the physical characteristics of char since the correlations used in this project for the physical properties of wood are not appropriate for temperatures greater than 373 K.

During pyrolysis the solid phase consists of both wood and char, with the mass of virgin wood decreasing and the mass of char increasing as pyrolysis progresses. Although Tran's kinetic expression for pyrolysis is for the rate of solid mass loss in general (solid species cannot be differentiated in thermogravimetric analyses) it is possible to isolate the production rate of char within the pyrolysis zone when a simplifying reaction model (the unreacted shrinking core model) is implemented. However, in this case, F_s, the flowrate of solid (wood and char) was chosen as the variable of interest in the pyrolysis zone. F_C, which in the absence of the above simplification is not well defined in this region, becomes important at the beginning of the combustion zone where all of the wood has been converted and any remaining solid is then char. (Even though it is meaningless in the drying and pyrolysis zones, F_C is initialized at the top of the bed as the fixed carbon fraction of the initial wood feedrate to facilitate its

introduction at a later stage in the computations.)

The energy balance is

$$\frac{d^2T}{dz^2} = \frac{\Sigma F_i C_{p_i} \, dT/dz + R_2 A' \Delta H_2 - 2\pi r \, h_w (T_a - T)}{k_e A'}$$

for $i = s, H_2O, H_2, CH_4, CO, CO_2, O_2, N_2$

2.3 Combustion

At some point along the length of the gasifier, air is injected into the packed bed. In the vicinity of the injection point there is a relatively large supply of oxygen and combustion can occur with hydrogen, methane, carbon monoxide and char all being potential fuels.

$$H_2 + 1/2\ O_2 \longrightarrow H_2O \qquad \text{Reaction (3a)}$$

$$CH_4 + 2\ O_2 \longrightarrow CO_2 + 2\ H_2O \qquad \text{Reaction (3b)}$$

$$CO + 1/2\ O_2 \longrightarrow CO_2 \qquad \text{Reaction (3c)}$$

$$\lambda C + O_2 \longrightarrow 2(\lambda-1)\ CO + (2-\lambda)\ CO_2 \qquad \text{Reaction (3d)}$$

2.3.1 Homogeneous Gas Phase Combustion

In the gasifier models developed to date homogeneous gas phase combustion of hydrogen, methane and carbon monoxide has been treated in different ways.

Yoon et al [1], in their model of the up-draft gasifier, report that although gas phase combustion of hydrogen and carbon monoxide may occur, the extent of reaction is not clear due to the short residence time of the gases in the packed bed. Calculations by Edgar et al [15] are cited as implying that the extent of reaction is insignificant. This does not appear to be a bad assumption for the up-draft gasifier since the oxygen/air blast contacts and reacts with the hot char long before it reaches the pyrolytic gases which are evolved near the top of the bed. However, in the down-draft gasifier the oxygen/air blast contacts both combustible gas and char simultaneously and the effect of

gas phase combustion is expected to be significant.

Tabatabaie-Raissi [3] does not include pyrolysis in his model of the down-draft gasifier. If the feedstock is considered to contain volatile material then the amount of this material is added to the predicted gasification product yields. There is no mention of gas phase combustion.

In Groeneveld's down-draft gasifier model [4] the oxygen in the combustion zone is considered to react with the pyrolysis gases to produce carbon dioxide and water. Any remaining oxygen then reacts with the char. The rates of these gas phase reactions are not considered; instead, these reactions are combined with pyrolysis in an overall calculation.

There is no information available on the homogeneous gas phase combustion of devolatilization products, probably due to the complexity of the reaction mechanisms as well as to the lack of need for such information [16]. However, in a recent paper [17] Reed and Markson describe a flaming pyrolysis region in a new down-draft gasifier design referred to as the stratified down-draft gasifier. In this design, both wood and air are fed to the top of the gasifier and, as a result, oxygen is present in excess in the pyrolysis zone. Combustion of the volatile gases which are evolved during pyrolysis has been observed as a flaming region surrounding each solid particle. This, clearly, is evidence for the importance of gas phase combustion in the down-draft gasifier.

2.3.2 Homogeneous Gas Phase Combustion Kinetics

In considering these gas phase reactions the extent of reaction depends on the chemical kinetics. Hottel et al [18] report the burning rate of carbon monoxide to be a

function of the oxygen, steam and carbon monoxide concentrations as well as of temperature and pressure.

$$R_{CO} = 12 \times 10^{10} \exp(-16000/RT)\, f_{O_2}^{0.3}\, f_{H_2O}^{0.5}\, f_{CO} \left[\frac{P}{RT}\right]^{1.8} \left[\frac{mol}{ml\ s}\right]$$

where $2 \times 10^{-7} < f_{H_2O} < 0.037$ (mol fraction)

$1.3 < N_2/O_2 < 9.07$ (molar basis)

$0.136 < \phi < 1.9$ (equivalence ratio)

$0.25 < P < 1$ atm

$1280 < T < 1535$ K.

The range of water concentration for which this correlation was devloped is too low for gasification studies. However, Hottel et al note that the effect of high water concentrations (>>0.10) is to decrease the exponent of the water mol fraction term to 0.4. The mol fraction of water in the volatile gases at the top of the combustion zone in the down-draft wood gasifier is typically greater than 0.10.

The temperature in the combustion zone is expected to exceed 1000°C (1273K) and Hottel's expression is appropriate for this region.

The reaction rate predicted by the above equation indicates that the homogeneous reaction often proceeds at more than ten times the intrinsic rate of the char combustion reaction. When mass transfer limitations are included for the solid-gas reaction the difference between the reaction rates is even greater. Calculations also show that, due to the low axial gas flow rate, the combustible gases will

react within approximately 1 mm in their progression down through the gasifier if there is sufficient oxygen available.

Furthermore, it is known that the combustion reaction rates decrease in the order hydrogen, methane, carbon monoxide, with the combustion of hydrogen being several orders of magnitude faster than the others. No appropriate kinetic information for the combustion of hydrogen and methane has been found in the literature. In the absence of this information hydrogen and methane combustion kinetics have been modelled by the carbon monoxide rate expression with f_{H_2} and f_{CH_4} being substituted for f_{CO}. Thus, the available oxygen at any position within the combustion zone is assumed to react with hydrogen, methane, carbon monoxide and char (see Section 2.3.3) simultaneously, but at different rates.

2.3.3 Char Combustion Kinetics

Sergeant and Smith [19] and Wicke and Wurzbacher [20] report the intrinsic rate of char combustion to be:

$$k_{r_3} = 1.79 \times 10^6 \exp(-27000/RT) \qquad \left(\frac{\text{mol } O_2}{\text{mol}_C \text{ atm s}}\right)$$

SERI [21] reports that the ratio of carbon monoxide to carbon dioxide produced during combustion has an important influence on the final product composition and the maximum temperature. Bhagat [22] has shown that this ratio is highly temperature dependent.

$$\left(\frac{CO}{CO_2}\right)_{\text{volume basis}} = 218 \exp\left(\frac{-7250}{T_s}\right)$$

where T_s is the temperature of the solid (K).

This correlation shows significant improvement over an

earlier correlation by Arthur [23].

2.3.4 Air Distribution Function

The rate of each of the combustion reactions depends on the local concentration of oxygen. Therefore, to model the combustion zone of the gasifier it is necessary to model the distribution of air within the packed bed.

In the Imbert gasifier design air is injected radially via a number of tuyeres which are positioned around the circumference of the gasifier. No information has been found in the literature which is appropriate for modelling this type of air jet geometry (which is further complicated by the presence of a packed bed and a perpendicularly flowing gas stream). The most appropriate model that we have found is for opposed jets in still air (no packed bed present). Becker and Ozum [24] recently examined the concentration fields generated by two opposed jets and reported their results as two-dimensional contours of concentration.

In our model, the movement of both solid and gas are assumed to be in plug flow, and thus all profiles are necessarily one-dimensional. Using a numerical integration technique, the two-dimensional concentration contours reported by Becker and Ozum were transformed into a one-dimensional concentration profile which is referred to as the air distribution function (Figure 6). This distribution function is used to determine the fraction of the total air feed which is injected at different axial positions in the bed, near the tuyere level.

When the effect of particle interference is considered, the concentration profile is expected to become less uniform

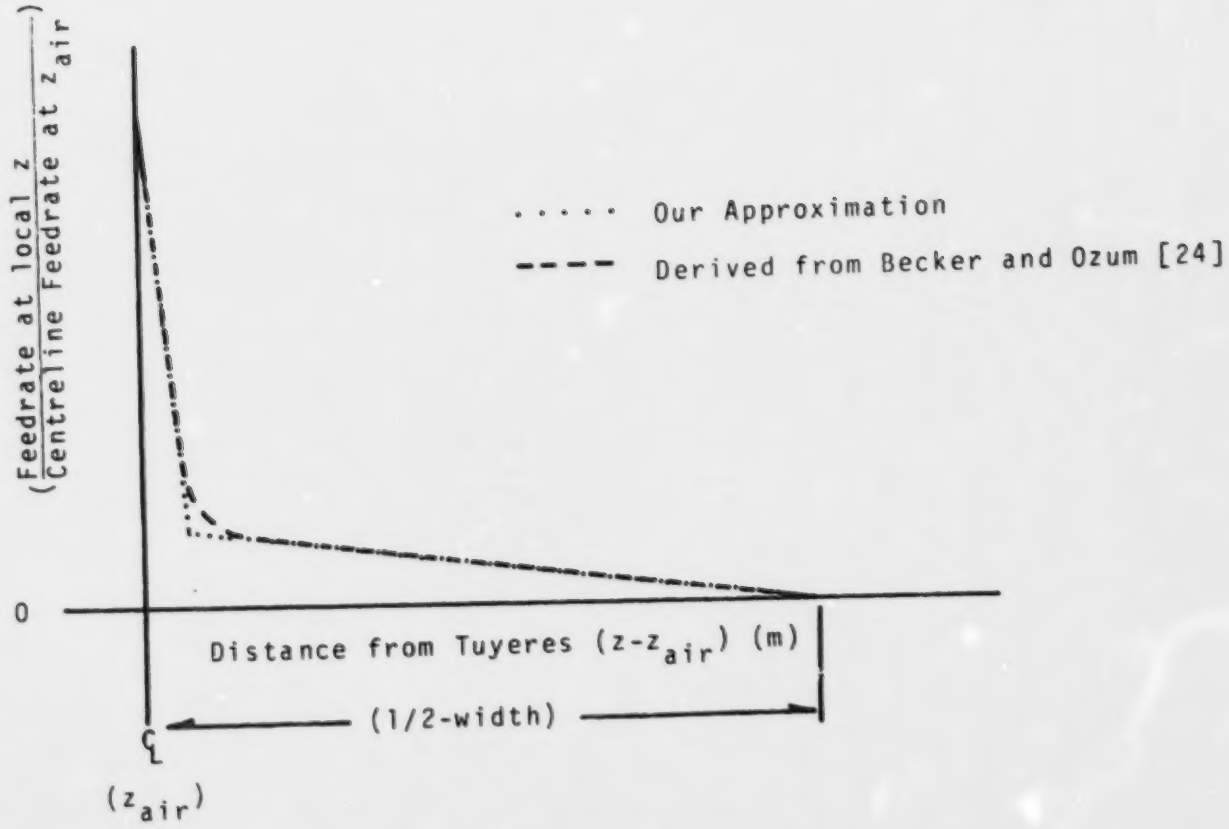

Figure 6 : The Air Distribution Function

radially (this is not considered in this model) and more dispersed axially. To account for the variation in dispersion an adjustable parameter w, the half-width of the air distribution zone, is introduced. Desrosiers [21] and Groeneveld [4] both report that oxygen is consumed within a few particle diameters of the air injection point, a distance of only a few centimeters. This suggests that w will be small (a value of 0.03 meters is used in the simulation). Finally, the skewing effect of the down-draft of gases from the pyrolysis zone is not included at this stage of model development.

2.4 Gasification

Gasification proceeds simultaneously with combustion where oxygen is present and by itself in the lower regions of the gasifier where there is no oxygen present. However, when the temperature falls below 750 °C the gasification reaction rates are very low, and gasification is considered to be halted. The following gasification reactions are assumed to proceed:

$$C + H_2O \longrightarrow CO + H_2 \qquad \text{(Reaction 4)}$$

$$C + CO_2 \longrightarrow 2\,CO \qquad \text{(Reaction 5)}$$

$$C + 2\,H_2 \longrightarrow CH_4 \qquad \text{(Reaction 6)}$$

Groeneveld [4] reports the following kinetic expressions for the reaction of wood char with steam and carbon dioxide:

$$k_{r_4} = 10^6\, C_C\, C_{H_2O}^{0.7} \exp(-26113/T) \qquad \left(\frac{\text{mol } H_2O}{m^3 s}\right)$$

$$k_{r_5} = 10^6 \, C_C \, C_{CO_2}{}^{0.7} \exp(-26113/T) \qquad \left(\frac{\text{mol } CO_2}{m^3 s}\right)$$

where C_C and C_{CO_2} are the concentration of solid char and gaseous carbon dioxide, respectively, (mol/m^3).

Tran's [11] results are used to model the hydrogasification of wood char. In a form similar to his pyrolysis model, where conversion now refers to the char and not to the wood, the rate of hydrogasification is computed as

$$-\frac{i}{W_1}\frac{dW}{dt} = k_6 \frac{W}{W_1} P_{H_2} \exp(-E_6/RT)$$

where $E_6 = E_6^\circ + a_1 X_1 + b_1 X_1^2$

$$X_1 = \frac{W_1 - W}{W_1}$$

W_1 is the total mass of char which is present before combustion commences

W is the mass of char remaining at time t

$-31 < a_1 < -3$ (kcal/mol)

$-83 < b_1 < -6$ (kcal/mol)

$2.7 \times 10^6 < k_6 < 7.5 \times 10^6$ ($min^{-1} atm^{-1}$)

$26 < E^\circ_6 < 33$ (kcal/mol)

In a form appropriate for use in this model,

$$k_{r_6} = 1.344 \times 10^7 \rho_s^\circ \frac{F_s^*}{F_s^\circ} (1 - X_1) \left(\frac{P_H}{P_{H_2} - P_{H_2}^{eq}} \right) \exp(\gamma)$$

where $\gamma = (13598 - 3422\ X_1 + 20100\ X_1^2)/T$

F_s^* is the solid mass flowrate after pyrolysis is complete

2.4.1 The Gas-Solid Reaction Model

The kinetic expressions provided so far are intrinsic rate expressions, appropriate for modelling reactions under carefully controlled conditions. However, in commercial operations with larger particle sizes such as those processed in down-draft gasifiers, it is necessary to consider the effects of mass transfer between gas and solid phases.

Several gas-solid reaction models which incorporate mass transfer effects have been proposed, including the shrinking unreacted core model(SCM), (of which the ash segregation model is a special case), the uniform conversion model, and more recently, volume reaction models. The shrinking core model is the simplest model and has been used extensively in gasifier modelling, notably by Yoon et al [1] in up-draft coal gasification modelling and by Desrosiers and Richey [2] in up-draft wood gasification modelling.

The volume reaction models are significantly more complex and their application to date has been limited. Groeneveld [4] justified his use of a volume reaction model by comparing predictions with the observed concentration profiles in samples of solid char. However, the nature of the experimental apparatus which he used leaves some doubt about whether the observed concentration profiles resulted only from diffusion through the particle slices or from shortcircuiting around the edges of the slices. Although the generality of the volume reaction model is useful since it includes both the shrinking unreacted core model and the uniform conversion model as extreme cases, there is no information in the literature from which the volume reaction

model parameters can be estimated. The complexity of the model makes it unattractive for use in this project.

Finally, the uniform conversion model has never been applied to wood gasification. This is understandable since, although Groeneveld's work does not prove beyond all doubt that the volume reaction model is necessary, the absence of uniform concentration profiles in his particle slices indicated that the uniform conversion model is not appropriate.

On the basis of the above considerations, a model of the shrinking unreacted core type was considered to be the most appropriate for wood gasification. Specifically, the ash segregation (AS) model is used, since the ash content of wood is very low (less that 0.2%). In the ash segregation model, reaction occurs only at the exterior surface of the particle and the unreacted core of the solid shrinks as reaction progresses. The solid ash which remains after reaction flakes off from the surface of the particle due to its low mechanical strength. The AS model includes the effects of mass transfer through a fluid film surrounding the solid particle and reaction at the solid surface. Developed for a spherical particle, the rate equation is:

$$R_i = \frac{(1-\varepsilon)(P_i - P_i^{eq})}{\frac{r_f L}{3k_p} + \left(\frac{P_i - P_i^{eq}}{k_{rj}}\right)} \qquad \left\{ \frac{mol_i}{m^3 s} \right\}$$

where ε = the void fraction in the packed bed

P_i = the partial pressure of gaseous reactant i

p_i^{eq} = the equilibrium partial pressure of reactant i

r_f = the fractional thickness of the particle compared

to the original particle dimensions

k_p = the film mass transfer coefficient

L = the half-thickness (radius) of the original particle

k_{rj} = the intrinsic reaction rate of reaction j

(The simulation program allows selection of either the SCM model or the AS model - FORTRAN code is included for both. See Appendix A.1.2)

The external mass transfer coefficient, k_p, has been reported by Gupta and Thodos [25] as

$$k_p = \frac{0.0038}{N_{Re}^{0.575}} \frac{G/M}{P_{gf}} \left(\frac{\mu m}{D_{i,mix}}\right)^{-2/3} \quad \left(\frac{mol_i}{m^2 s\ atm}\right)$$

where G = the superficial gas mass velocity (kg/s m^2)

P_{gf} = partial pressure of the non-transferable component in the gas film (atm)

This correlation is recommended for $90 < Re < 4000$, which is appropriate for the down-draft gasifier.

2.4.2 Mass and Energy Balances for the Combustion and Gasification Zones

The differential equations which govern behaviour in the combustion zone are:

$$\frac{dF_s}{dz} = \frac{dF_C}{dz} = -(\lambda R_{3d} + R_4 + R_5 + 1/2\ R_6)\ M_C A'$$

$$\frac{dF_{H_2O}}{dz} = (R_{3a} + 2R_{3b} - R_4)\ M_{H_2O}\ A' + g_{H_2O} F^{\circ}_{air}$$

$$\frac{dF_{H_2}}{dz} = (-R_{3a} + R_4 - R_6)\ M_{H_2} A'$$

$$\frac{dF_{CH_4}}{dz} = (-R_{3b} + 1/2\ R_6)\ M_{CH_4} A'$$

$$\frac{dF_{CO}}{dz} = (-R_{3c} + 2(\lambda-1)R_{3d} + R_4 + 2\ R_5)\ M_{CO} A'$$

$$\frac{dF_{CO_2}}{dz} = (R_{3b} + R_{3c} + (2-\lambda)R_{3d} - R_5)\ M_{CO_2} A'$$

$$\frac{dF_{O_2}}{dz} = -(1/2\ R_{3a} + 2\ R_{3b} + 1/2\ R_{3c} + R_{3d})\ M_{O_2} A' + g_{O_2} F^{\circ}_{air}$$

$$\frac{dF_{N_2}}{dz} = g_{N_2} F^{\circ}_{air}$$

F°_{air} is the local air flowrate which is determined according to the air distribution ($kg_{air} s^{-1} m^{-1}$). g_{H_2O}, g_{O_2}, and g_{N_2} are the mass fractions of water, oxygen and nitrogen, respectively in the "air" feed to the gasifier.

The energy balance is:

$$\frac{d^2T}{dz^2} = [(\sum F_i C_{pi}\, dT/dz) + (R_{3a}\Delta H_{3a} + R_{3b}\Delta H_{3b} + R_{3c}\Delta H_{3c} + R_{3d}\Delta H_{3d} + R_4\Delta H_4 + R_5\Delta H_5 + R_6\Delta H_6)A' - 2\pi r\, h_w(T_a - T)] / (k_e A')$$

for i = C, H_2O, H_2, CH_4, CO, CO_2, O_2, N_2

The gasification zone model is almost identical to that of the combustion zone, except that reactions 3a,b,c,d do not occur. The differential equations describing this zone are:

$$\frac{dF_s}{dz} = \frac{dF_C}{dz} = -(R_4 + R_5 + 1/2\ R_6)\ M_C A'$$

$$\frac{dF_{H_2O}}{dz} = -R_4\ M_{H_2O}\ A'$$

$$\frac{dF_{H_2}}{dz} = (R_4 - R_6)\ M_{H_2} A'$$

$$\frac{dF_{CH_4}}{dz} = 1/2\ R_6\ M_{CH_4}\ A'$$

$$\frac{dF_{CO}}{dz} = (R_4 + 2\ R_5)\ M_{CO}\ A'$$

$$\frac{dF_{CO_2}}{dz} = -R_5 M_{CO_2} A'$$

$$\frac{dF_{O_2}}{dz} = \frac{dF_{N_2}}{dz} = 0.$$

The energy balance is:

$$\frac{d^2T}{dz^2} = [(\Sigma F_i C_{pi} dT/dz) + (R_4 \Delta H_4 + R_5 \Delta H_5 + R_6 \Delta H_6) A' - 2\pi r\, h_w (T_a - T)]/(k_e A')$$

The variation of $\Sigma F_i C_{pi}$ throughout the gasifier is small and is considered negligible in the development above (see Section 2.6).

2.5 The Post-Reaction Zone

2.5.1 Mass and Energy Balances for the Post-Reaction Zone

In the post-reaction zone the gases cool and it is assumed that no further reaction occurs. The differential equations describing this zone are:

$$\frac{dF_i}{dz} = 0 \qquad \text{for } i = C_{H_2O},\ H_2,\ CH_4,\ CO,\ CO_2,\ O_2,\ N_2$$

The energy balance is:

$$\frac{dT}{dz} = \frac{-2\pi[r_w h_w (T-T_c) + r_o h_{wo} (T-T_{amb})]}{\Sigma(F_i C_{pi})}$$

$$\frac{d^2T}{dz^2} = 0$$

Note that T is the local temperature, so that for computation in the annulus T becomes the updated value of T_a. For computing the heat transfer driving force T_c is the temperature of the packed bed at the same axial position, and T_{amb} is the ambient temperature. h_w is the overall heat transfer coefficient between the annulus and the packed bed while h_{wo} is the overall heat transfer coefficient between the annulus and the ambient environment.

2.6 The Energy Balance

The energy balance for a differential compartment within the gasifier accounts for:

i) heat transfer by convection of solid and gas in the direction of bulk flow

ii) axial heat transfer including both conduction and radiation effects

iii) heat transfer radially through the gasifier walls

iv) heat generation by chemical reaction, evaporation and devolatilization

The heat capacity of the gas/solid mixture does not change rapidly along the length of the gasifier. Therefore, only periodic updating of the physical properties such as heat capacities is performed. The convective heat flux, $\Sigma F_i C_{p_i}$, also does not vary strongly with position in the gasifier. Therefore, considering the convective heat flux to be approximately constant across a differential element, at steady state these combined effects give

$$-k_e A' \frac{d^2T}{dz^2} + \left(\sum_i F_i C_{pi} \right) \frac{dT}{dz} + R_j \Delta H_j A' - 2\pi r h_w (T_a - T) = 0$$

Separating this second order differential equation into two coupled first order differential equations gives

$$\frac{dT}{dz} = U$$

$$\frac{dU}{dz} = \frac{d^2T}{dz^2} = \frac{(\sum_i F_i C_{pi})U + \Sigma R_j \Delta H_j A' - 2\pi r h_w (T_a - T)}{k_e A'}$$

2.6.1 Axial Heat Transfer

Yagi and Kunii [26] present a formulation for estimation of the effective axial thermal conductivity in a packed bed which includes:

i) heat transfer through the solid particle

ii) heat transfer through solid-solid surface contact

iii) radiant heat transfer from solid to solid surfaces

iv) radiant heat transfer between adjacent voids

v) heat transfer through the fluid film near the contact surface

vi) heat transfer by convection, solid-fluid-solid

vii) heat transfer by lateral mixing

$$k_e = k_e^\circ + \alpha\beta\, k_g\, N_{Pr} N_{Re}$$

where $$k_e^\circ = \frac{\beta\,(1-\varepsilon) k_g}{\left(\frac{\gamma k_g}{k_s} + \frac{1}{\frac{1}{\phi} + \frac{d_p h_{rs}}{k_g}}\right)} + \varepsilon\beta\, d_p\, h_{rv}$$

$$h_{rs} = 0.1952 \left(\frac{\varepsilon_m}{2-\varepsilon_m}\right) \left(\frac{T}{100}\right)^3$$

$$h_{rv} = \frac{0.1952}{1 + \left(\frac{\varepsilon}{2(1-\varepsilon)}\right)\left(\frac{1-\varepsilon_m}{\varepsilon_m}\right)} \left(\frac{T}{100}\right)^3$$

where k_e = the effective axial thermal conductivity (kcal/m hr °C)

$k_e°$ = the effective thermal conductivity in the packed bed with motionless fluid (kcal/m hr °C)

k_g = the thermal conductivity of the fluid (kcal/m hr °C)

k_s = the thermal conductivity of the packing material (kcal/m hr °C)

h_{rs} = the heat transfer coefficient for radiation, solid to solid (kcal/m^2 hr °C)

h_{rv} = the heat transfer coefficient for radiation, void to void (kcal/m^2 hr °C)

ε_m = the solid emissivity

ε = the void fraction in the packed bed

T = the local temperature (K)

d_p = the particle diameter (m)

α = mass velocity of fluid flowing in the direction of heat or mass transfer/mass velocity of fluid based on sectional area of empty tube in the direction of fluid flowing

β = effective length between centres of particles/ nominal particle diameter = l_p/D_p

Yagii and Kunii suggest

$$\alpha\beta = 0.14$$

$$0.82 < \beta < 1.0$$

$$\gamma = 1.0$$

$$\phi = 0.034 \qquad \text{for } \varepsilon = 0.4$$

For wood char the emissivity, ε_m, is approximately 0.95.

2.6.2 Heat Transfer Through the Gasifier Walls

In heat transfer through the walls of the gasifier three

steps occur in series:

i) transfer from the packed bed to the wall

ii) conduction through the wall, and

iii) transfer from the wall to the environment on the external side of the wall

When the gasifier has concentric regions, e.g. packed bed surrounded by an annulus as in the Imbert gasifier, the situation is more complicated. However, the wall heat transfer component of the energy balance for any particular compartment in the gasifier model involves only three contributions.

$$h_w = \frac{1}{\frac{A_o}{A_i h_i} + \frac{A_o \Delta r}{A_{lm} k_w} + \frac{1}{h_o}}$$

The following heat transfer correlations have been used:

* Transfer from the packed bed to the wall [27]

$$h_{pb} = 0.813 \frac{k_g}{d_t} e^{-6d_p/d_t} N_{Re}^{0.9} \qquad \text{for } \left\{\frac{d_p}{d_t}\right\} < 0.35$$

* Transfer from the inner wall to the annulus and from the annulus to the outer wall [28]

$$h_{ia} = 1.02 \frac{k_g}{d_e} N_{Re}^{0.45} N_{Pr}^{0.5} \left(\frac{d_e}{L}\right) \left(\frac{d_2}{d_1}\right)^{0.8} \left(\frac{\mu_b}{\mu_l}\right)^{0.14} N_{Gr}^{0.05}$$

for $N_{Re} < 2100$

$d_e = d_2 - d_1$

$$d'_e = \frac{d_2 + d_i}{2}$$

* Transfer by natural convection from the outer wall of the gasifier to the ambient environment [29]

$$N_{Nu} = 0.138\ N_{Gr}^{0.36}\ (N_{Pr}^{0.175} - 0.55) \qquad \text{for } N_{Gr} < 10^9$$

$$= 0.683\ N_{Gr}^{0.25}\ N_{Pr}^{0.25} \left\{ \frac{N_{Pr}}{0.861 + N_{Pr}} \right\}^{0.25} \qquad \text{for } N_{Gr} > 10^9$$

for $1 < N_{Pr} < 40$.

* Thermal conductivity of the gasifier wall [30]

$k_w = 50$ ($\frac{J}{s\,m\,K}$) for carbon steel

2.6.3 Heat Generation by Reaction

The heat generation associated with each reaction is computed from the data in Tables 3 and 11 (Appendix A.2), and the heat of pyrolysis is computed as shown in Section 2.2.3.

2.7 ANALYSIS OF THE MECHANISTIC MODEL

Our analysis of the mechanistic model has three components : analysis of the computational behaviour of the model itself, analysis of the sensitivity of the predicted results to the model parameters and finally, comparison of the model predictions with actual down-draft gasifier operational data (provided by Saskatchewan Power Corporation (SPC)). In presenting the analysis no attempt is made to separate these elements for they complement each other in the process of model evaluation.

2.7.1 Initial Values

The differential equation solution package DGEAR [31] requires initial values for each of the eleven dependent variables: F_s, F_C, F_{H_2O}, F_{H_2}, F_{CH_4}, F_{CO}, F_{CO_2}, F_{O_2}, F_{N_2}, T and dT/dz.

The initial values which have been chosen are listed below (numerical values used in this particular simulation are listed in Appendix A.3).

F°_s = feedrate of wet wood (kg/s)

F°_C = fixed carbon fraction of initial feedrate of wet wood (kg/s)

$F^\circ_{H_2O}$ = flowrate of water vapour in saturated air entering with the wood at the initial temperature (kg/s)

$F^\circ_{H_2} = F^\circ_{CH_4} = F^\circ_{CO} = F^\circ_{CO_2} = 0$ (kg/s)

$F^\circ_{O_2}$ = feedrate of oxygen trapped in void spaces

between wood particles at initial feeding (kg/s)

$F^{\circ}_{N_2}$ = feedrate of nitrogen trapped in void spaces between wood particles at initial feeding (kg/s)

T° = temperature at the top of the bed at steady state (K)

$(dT/dz)^{\circ}$ = rate of change of temperature with axial position at the top of the bed at steady state (K/m)

All of the initial values, except T° and $(dT/dz)^{\circ}$, are computed directly from the selected operating conditions. These latter two values are only estimates and they are changed if the boundary condition at the bottom of the gasifier is not satisfied at the end of a profile iteration.

2.7.2 Simulated Results: Drying and Pyrolysis

2.7.2.1 The Temperature Profile

Using the above set of initial values, the prediction of the temperature profile in the upper regions of the down-draft gasifier appears reasonable (Figure 7). At the top of the bed the temperature increases very slowly for the first 0.5 meters. Numerically, the temperature varies little at the top because the initial value of $(dT/dz)^{\circ}$ is low. Furthermore, the heat transfer to this region is low enough that (dT/dz) does not increase rapidly.

The initial temperature T° is expected to be above ambient temperature yet at or below 373 K (the boiling point of water at one atmosphere). Data supplied by Saskatchewan Power suggest that an initial value of 373K is reasonable. Two thermocouples placed on the outside surface of the inner wall of the gasifier near the top of the bed (measurements 001 and 007 in Table 15, Appendix A.4) show that the

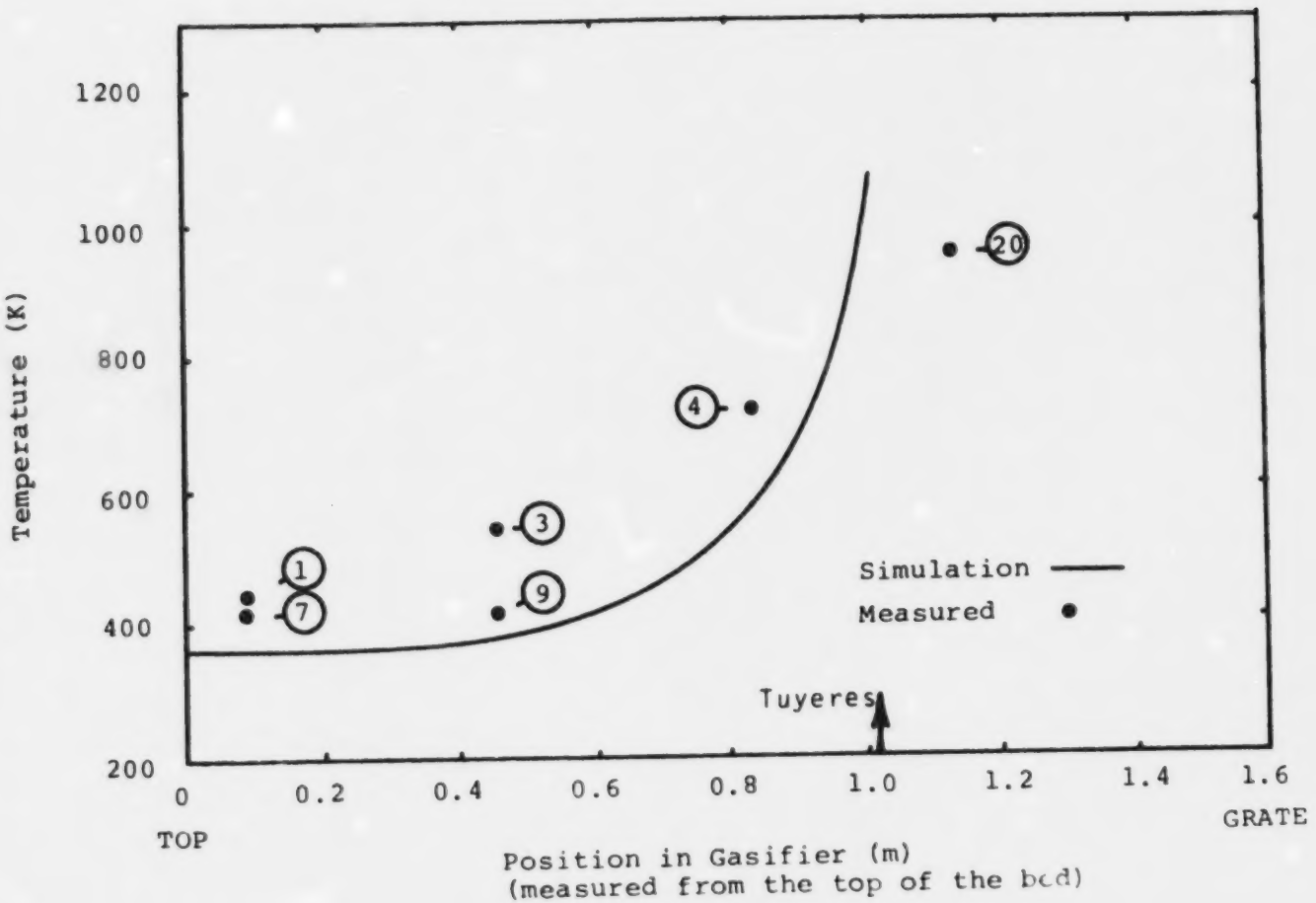

Figure 7 : Comparison of the Simulated Temperature Profile with SPC Temperature Measurements

temperature at this point is approximately 150°C (423K). At the top of the gasifier the temperature in the annulus is expected to be higher than in the centre of the bed and therefore the predicted temperature in the bed is expected to be less than these measured values.

The temperature rises as drying proceeds, due to heat transfer through the wall and axial conduction from the hotter regions in the gasifier. Drying is complete in 0.8 to 0.9 meters from the top of the bed and at this point pyrolysis commences. The temperature at the boundary between the drying and pyrolysis zones is approximately 360°C (633 K). Wide variations ($\pm$ 10%) in T°, (dT/dZ)°, the wood feed rate and wood moisture content have little effect on this temperature (Table 4).

Shafizadeh [32] reports that there is negligible weight loss due to pyrolysis at temperatures below 270°C. Between 270°C and 310°C he reports an initiation period in the weight loss, and above 310°C a first order rate of weight loss. Therefore, by requiring that pyrolysis commence only after drying is complete we are ignoring the potentially significant weight loss from 310 to 360°C. However, according to our predictions the distance between points in this region of the gasifier at 310 and 360 °C is less than 0.05 meters. Since this is not a critically high temperature region such a difference will not be of concern in gasifier design.

The SPC data include temperature measurements in this general location (middle to end of drying zone) (measurements 3, 9 and 4 in Figure 7). Here again, the predicted temperature is slightly lower than the measured wall temperatures indicate, as is expected. However, the measured (425K,540K) and predicted (410K) temperatures are close.

Complete pyrolysis of the dry wood requires a distance of only 0.1 meters in the bed. The extent of the pyrolysis zone is affected very little by variation of T°, (dT/dZ)° the wood feedrate or the wood molsture content (Table 4). in conjunction with the drying zone as described above and subject to the selected initial values of T and (dT/dz), this indicates that both drying and pyrolysis are complete before oxygen is contacted in the vicinity of the tuyeres. The pyrolysis zone is very close to the high temperature combustion zone and, due largely to axial conduction and radiation, the temperature rises very quickly in a very short distance. At the end of the pyrolysis zone (dT/dz) is approximately 5000 K/m and the temperature is approximately 1000 K.

There are no SPC temperature measurments in this narrow pyrolysis region. The next measurement (020 in Figure 7) is located beyond the tuyere level, in the combustion region.

The sensitivity of the simulated results to the initial temperature is shown in Figure 8. For a larger value of T° a longer distance in the bed is required for the wood to dry. This can be attributed to the temperature difference which is the driving force for heat transfer across the gasifier walls. The same annular temperature profile has been used in each of these simulations. Therefore, the lower T° is, the greater is the temperature difference across the wall. Continuing the same line of argument, the greater is the heat flux across the wall and the faster the wood dries. This odd behaviour should disappear when the simulated profile calculations are iterated to convergence. The profiles reported in this paper are "first iteration" profiles only. Due to numerical difficulties (see Section 2.7.4) final converged profiles have not been obtained.

Table 4 : Sensitivity Analysis of the Pyrolysis Zone - Location and Temperature

Basic test case conditions : T^{o} = 373 K
$(dT/dz)^{o}$ = 1.0 K/m
Moisture = 0.15 (dry basis)
Wood Feedrate = 0.02 kg/s (wet basis)

Variable Adjusted	To a value of	Pyrolysis commences @ Location (m)	Pyrolysis commences @ Temperature (K)	Pyrolysis ends @ Location (m)	Pyrolysis ends @ Temperature (K)
None	------	0.89	631	1.00	998
T^{o}	350	0.83	613	0.95	987
T^{o}	320	0.77	633	0.86	947
$(dT/dz)^{o}$	0.0	----	---	----	----
$(dT/dz)^{o}$	0.8	0.91	621	1.02	1020
$(dT/dz)^{o}$	1.2	0.87	631	0.99	1010
$(dT/dz)^{o}$	10.	0.65	644	0.76	956
F_s^{o}	0.022	0.81	619	0.92	952
Moisture	0.20	0.89	630	1.00	991
Moisture	0.25	0.91	666	1.00	977

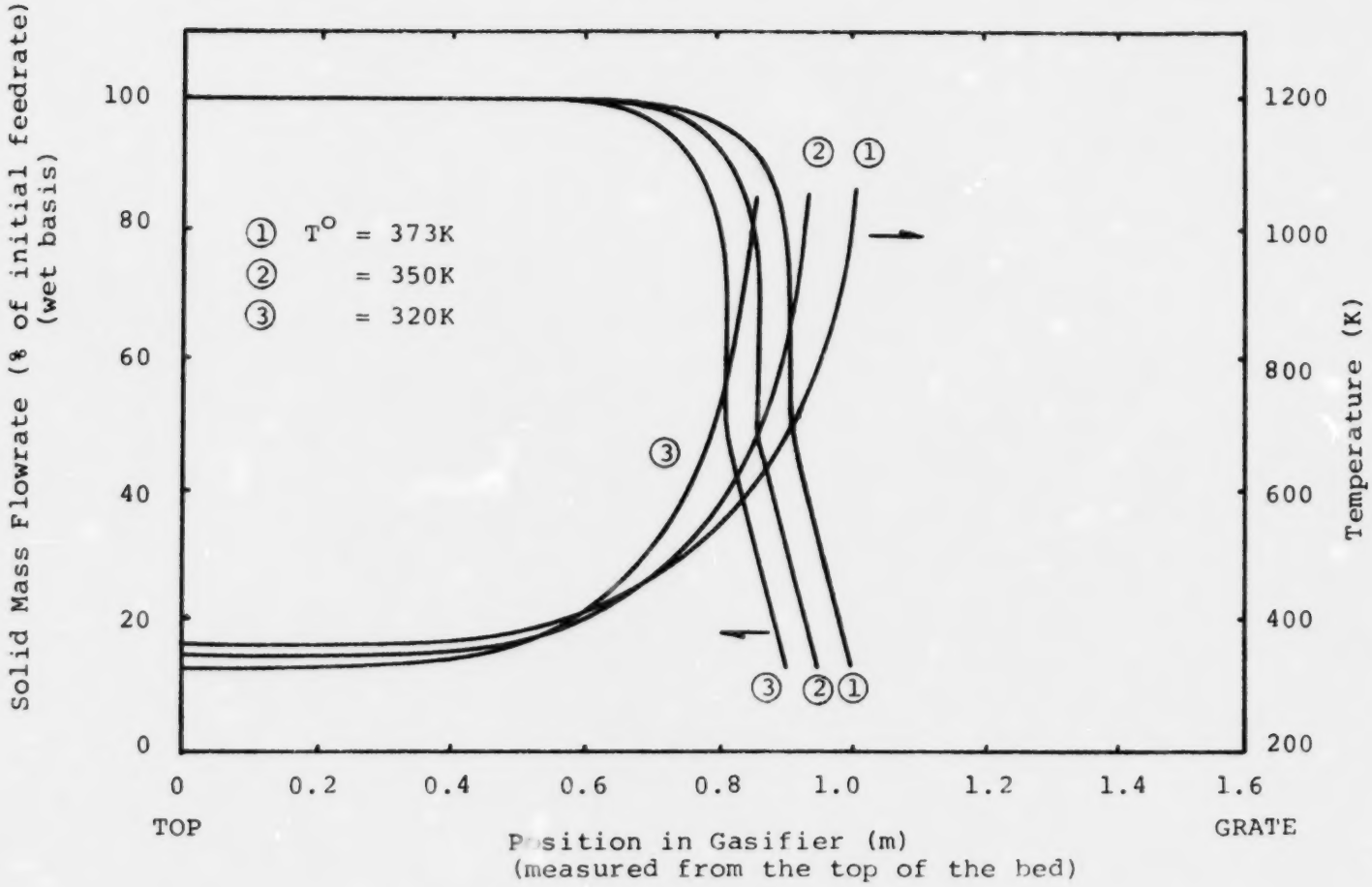

Figure 8 : The Effect of T^{O} on the Simulated Results

The initial value of (dT/dz) is a critical factor in the simulation program. A value of unity for (dT/dZ)° has been used in computing the results presented in this report. However, Figure 9 shows the sensitivity of the simulation to this value. Initially it was expected that (dT/dz)° should be zero at the top of the bed. However, under this condition the predicted temperature drops monotonically, an unreasonable prediction for gasifier operation. A small variation in (dT/dz)° about unity results in a variation in the length of the drying zone - the higher (dT/dz)° is, the shorter is the distance required for complete drying, as is expected.

2.7.2.2 The Composition Profile

The solid mass flowrate decreases very slowly in the upper 0.8 meters of the gasifier, the region in which the increase in the temperature is very small . Only when the temperature starts to increase significantly is there a noticeable decrease in the solid mass flowrate (Figure 8) due to the evaporation of water from the wood. Once pyrolysis commences the solid mass flowrate drops rapidly, the rate of decrease slowing somewhat as conversion increases. Conversion is found to exceed 50% in a very short distance and, as suggested by Mackay and Roberts [12], this is achieved before the temperature reaches 500°C.

The composition of the gas phase is shown in Figure 10 (note the abbreviated abscissa), where the presence of each species is indicated by its partial pressure. The composition of the gas at the top of the bed (not shown in Figure 10) is that of air saturated with water vapour at T^{o}. As drying progresses the partial pressure of water increases and eventually predominates and the oxygen and nitrogen partial pressures become negligible. Although the oxygen

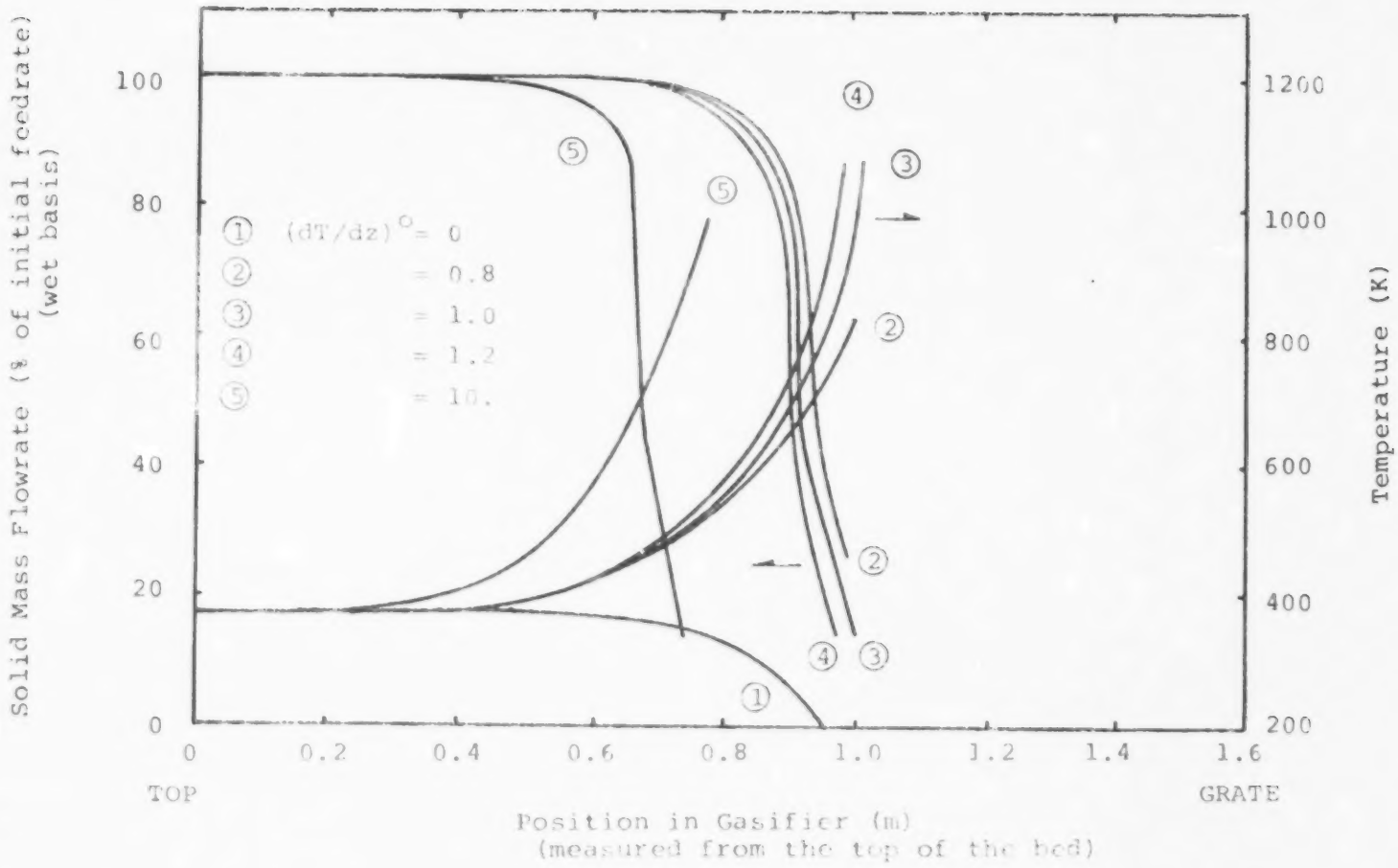

Figure 9 : The Effect of $(dT/dz)^{o}$ on the Simulated Results

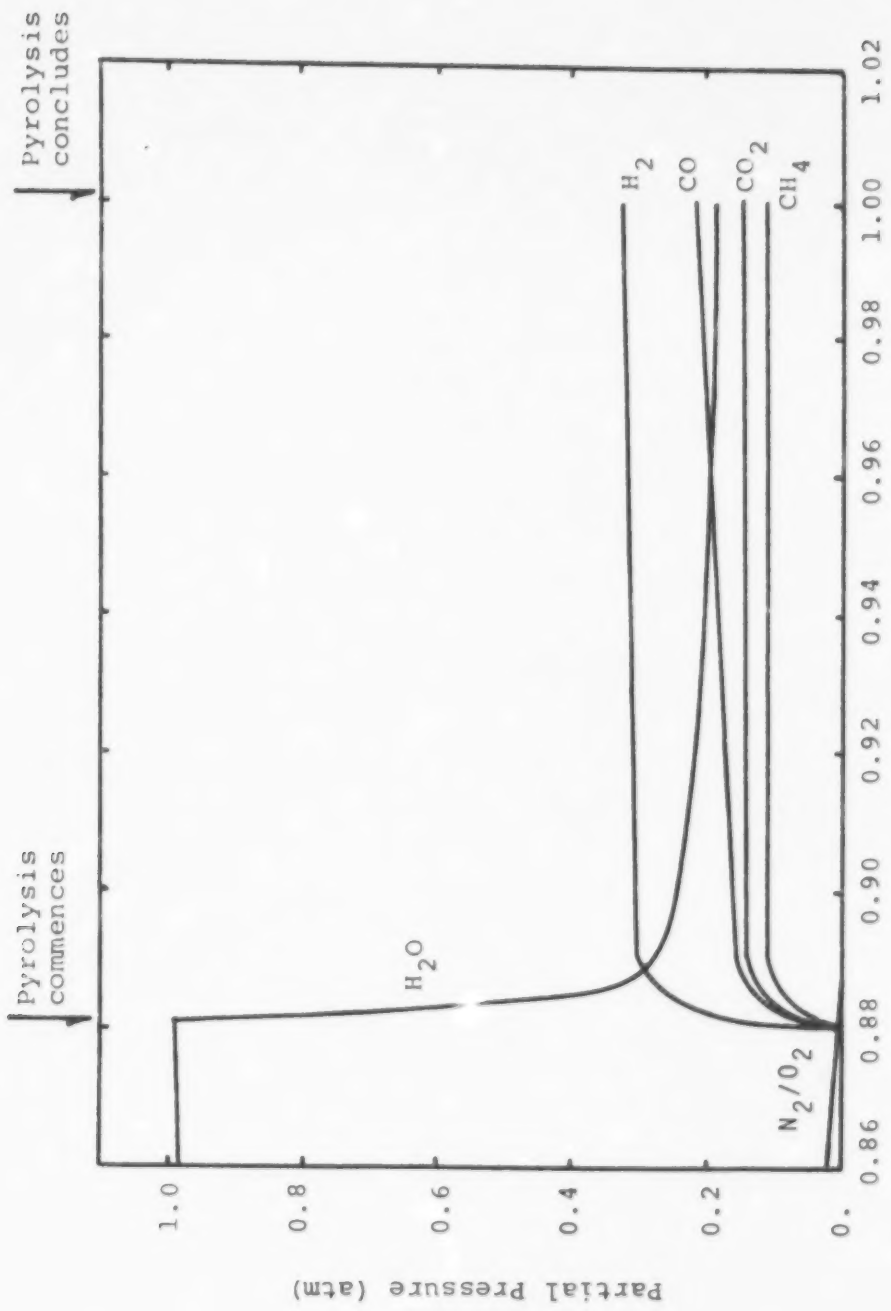

Figure 10 : Gas Composition in the Pyrolysis Zone

and nitrogen flowrates themselves do not decrease, the evolution of water vapour causes the total gas flowrate to increase dramatically, and the original oxygen and nitrogen flowrates become negligible in comparison.

At the beginning of the pyrolysis zone hydrogen, methane, carbon monoxide and carbon dioxide begin to appear. Because a large fraction of the pyrolysis is complete in the very early stages of the pyrolysis region the distribution of these products is largely dependent on the initial temperature in this region. The partial pressures of each of these products varies little after this initial pyrolysis.

Sensitivity of the solid mass flowrate profile to T° and $(dT/dz)^\circ$ is also shown in Figures 8 and 9. The observations are similar to those for the temperature profile. In this case, the lower T° is and the higher $(dT/dz)^\circ$ is, the shorter is the distance required for drying. We offer the same explanation as before for the unexpected behaviour with respect to the selection of T°.

As shown in Table 5, variations in T° and $(dT/dz)^\circ$ have no effect on the composition of the gas at the end of the pyrolysis zone, since the initial temperature of pyrolysis is approximately the same (633K) in all cases.

In their recent report [33] Saskatchewan Power provided a qualitative cross-sectional representation of their Imbert gasifier (Figure 11). Based on observations made during emptying of the gasifier after extended periods of operation they noted the state of the solid particles at different locations in the bed. This schematic indicates that:

1. wet wood is still present at a point approximately 1 meter from the top of the bed

Table 5 : Sensitivity of the Pyrolysis Zone - Gas Composition at the End of the Zone

Variable Adjusted	To a value of	Gas Composition (partial pressure - atm) H_2O	H_2	CH_4	CO	CO_2	N_2
None	-----	0.192	0.324	0.121	0.204	0.158	0.001
T^o	350	0.191	0.325	0.121	0.202	0.160	0.001
T^o	320	0.190	0.325	0.121	0.202	0.160	0.002
$(dT/dz)^o$	0.0	-----	-----	-----	-----	-----	-----
$(dT/dz)^o$	0.8	0.193	0.323	0.121	0.205	0.158	0.000
$(dT/dz)^o$	1.2	0.192	0.324	0.121	0.203	0.159	0.001
$(dT/dz)^o$	10.	0.190	0.325	0.121	0.201	0.161	0.002
F_s^o	0.022	0.191	0.325	0.121	0.202	0.160	0.001
Moisture	0.20	0.234	0.307	0.115	0.193	0.150	0.001
Moisture	0.25	0.272	0.292	0.109	0.184	0.14[illegible]	0.000

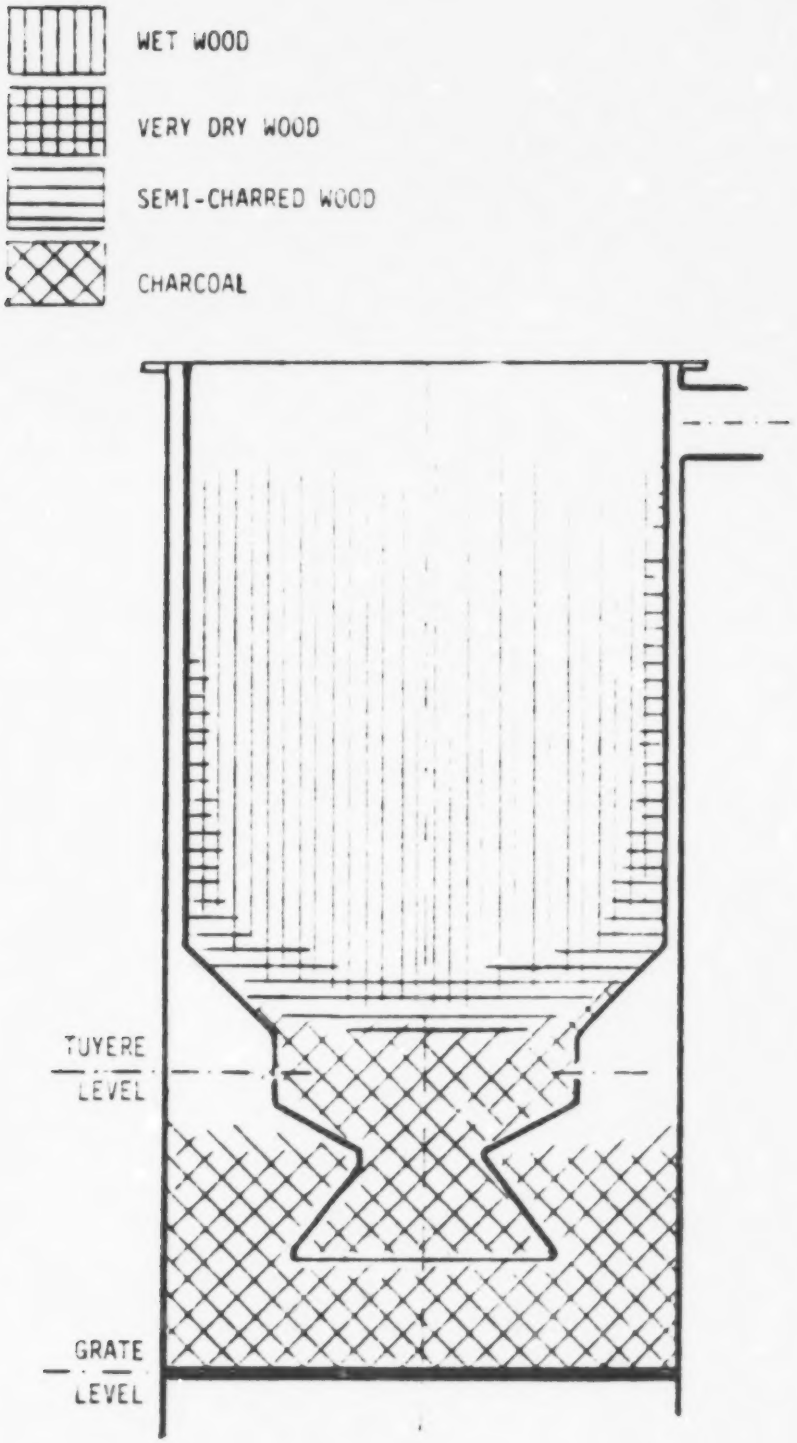

Figure 11 : SPC Gasifier Cross-Section
Conversion of Wood and Char [33]

2. charring of the wood requires a relatively short distance of approximately 0.1 meters, and is complete at less than 0.1 meters above the centre-line of the tuyeres.

The fact that the input conditions used for the simulation are similar to the SPC operating conditions (including particle size, moisture content and wood feedrate), provides further support for our model predictions, indicating that the models for the rates of drying and pyrolysis are appropriate for the down-draft gasifier. A more complete evaluation of the validity of these models, particularly of the predicted gas composition, requires more extensive experimental measurements of temperature and composition in these regions.

2.7.2.3 Problems with the Pyrolysis Model

Although the kinetic part of the pyrolysis model produced reasonable predictions of the extent of the pyrolysis zone in the gasifier, considerable difficulty was encountered in attempting to describe the full pyrolytic product distribution given only the dry gas distributions available in the literature.

The first assumption which was made in developing the pyrolytic product distribution was that the volatiles are evolved from the wood particle in a shrinking core manner (see Section 2.2.1). This assumption required that the overall atomic composition of the volatiles evolved at any time be the same as the overall atomic composition which was computed from the proximate and ultimate analyses (Appendix A.1.1). In the early stages of this project we used proximate and ultimate analyses for a white spruce feedstock which were reported in the literature [53].

When the dry gas product distributions (relative amounts of H_2, CO, CH_4 and CO_2) were combined with the overall atomic composition criterion above, some of the element balances would not close. This suggested that there were other devolatilization products formed in the dry gas distribution studies although they were not reported. We introduced H_2O and a pure carbon char (C) to the model in an attempt to make the balances close.

With some manipulation and qualitative interpretation of the available dry gas distributions we found values for R_H (equation 5, Section 2.2.1) which when used with the other product distribution equations, gave reasonable predictions of a "full" pyrolysis product distribution which included C, H_2O, H_2, CH_4, CO and CO_2. This "full" product distribution showed the same general characteristics as the dry gas distribution except for an unusually high prediction of H_2 yield which stemmed from our assumption of a pure carbon char.

Later in our work, we obtained an experimental determination of the proximate and ultimate analyses of the white spruce feedstock that was being used in the operation of the Saskatchewan Power gasifier. When these new analyses were substituted for the literature values in our product distribution model our element balances again failed to close. Further adjustment of R_H was necessary. Although the resulting distribution (Fig. 3) still shows the general characteristics of the dry gas distribution (except for H_2 again) the appropriateness of this type of adjustment of R_H to satisfy different feedstock analyses is uncertain.

Later, another analysis of a sample of the SPC feedstock was performed at Queen's University. Again, although the ultimate analysis is similar to the literature value and to the

SPC results, a very different proximate analysis was recorded.

Table 5a: Proximate and Ultimate Analysis of White Spruce

		[53]	SPC	Queen's
Ultimate Analysis (wt% dry basis)	C	.441	.492	.478
	H	.056	.061	.060
	O	.494	.444	.446
	N	.001	.000	.000
	Ash	.008	.003	.016
Proximate Analysis (wt% dry basis)	fixed carbon	.198	-	.124
	volatiles	.794	-	.861

However, until more definite analytical techniques are developed this problem cannot be resolved. The "full" pyrolytic product distribution that we have developed appears reasonable when compared to the dry gas distribution information, however its adequacy for gasifier modelling will be unknown until gas samples are extracted from the interior of an operating gasifer for comparison.

2.7.3 Simulated Results: Combustion and Gasification

The results of this simulation are shown in Figure 12. As soon as the combustion zone is reached the very high exotnermicity of the combustion reactions overwhelms all other heat transfer contributions. However, the simulated results show very large, negative values of dT/dz. As a result, the temperature drops quickly to zero, an unrealistic condition.

Consider the following analysis:

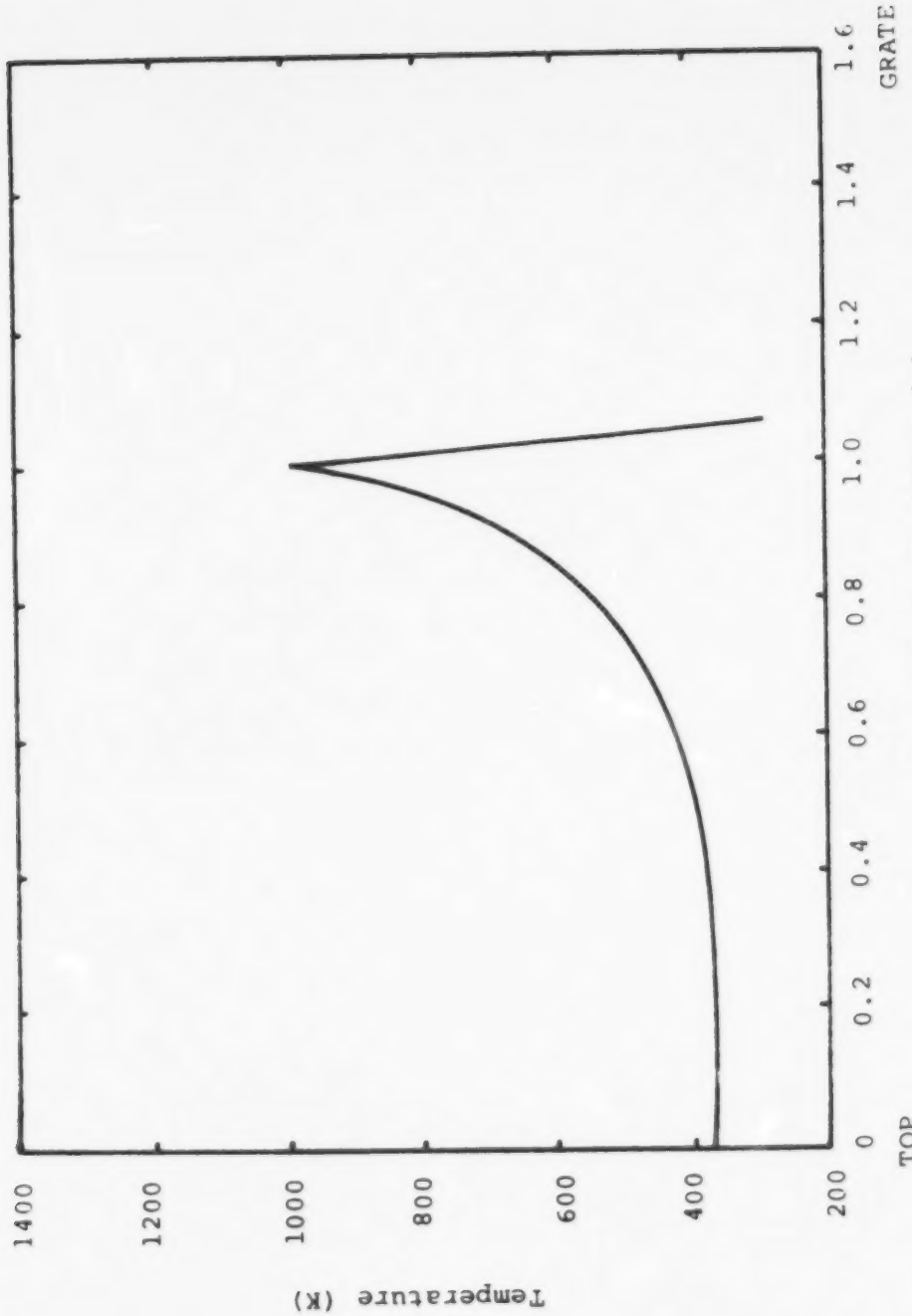

Figure 12 : Simulated Temperature Profile

Table 6a: Expected Temperature Profile Characteristics
(no axial conduction)

Zone	$-\Sigma R_j \Delta H_j A'$	$2\pi r h_w (T-T_a)$	dT/dz	Reason
Drying	small −	small +	small +	endothermic
Pyrolysis	med −	small +	med +	endothermic
Combustion	large +	−	large +	exothermic
	med +	−	small +	oxygen depletion
	small +	−	small −	" "
Gasification	med −	−	large −	oxygen gone
	small −	−	med −	temperature low
Post-Reaction	0	−	small −	temperature 750°C
	0	0	0	

Table 6b: Expected Temperature Profile Characteristics
(including axial conduction)

Zone	$\Sigma R_j \Delta H_j A'$	$-2\pi r h_w (T-T_a)$	$\Sigma F_i C_{pi} dT/dz$	d^2T/dz^2
Drying	small +	small −	small +	+
Pyrolysis	med +	small −	med +	+
Combustion	large −	+	large +	+
	med −	+	small +	−
	small −	+	small −	−
Gasification	med +	+	large −	−
	small +	+	med −	−
Post-Reaction	0	+	small −	−
	0	0	0	0

If there was no solid bed present in the gasifier (gas phase combustion would still proceed) then the axial thermal conduction would be negligible. The resulting energy balance would have the form:

$$\frac{dT}{dz} = \frac{-\Sigma R_j \Delta H_j A' + 2\pi r h_w (T-T_a)}{\Sigma F_i C_{pi}}$$

Knowing the nature of the contributions in the numerator for each of the reaction zones, the conclusions in Table 6a can be deduced.

Extending these ideas to the case where axial conduction is important we would expect the behaviour noted in Table 6b.

$$\frac{d^2T}{dz^2} = \frac{\Sigma F_i C_{pi} dT/dz + \Sigma R_j \Delta H_j A' - 2\pi r h_w (T-T_a)}{k_e A'}$$

(Note that the signs have changed since the terms change sides in the energy balance equation.)

Therefore, the temperature profile is expected to have the form shown in Figure 13, as the SPC temperature measurements show. Note that the maximum temperature is reached before the end of the combustion zone, due to the growing importance of the gasification reactions and the decreasing importance of the combustion reactions.

It has been noted that the behaviour of the temperature profile is very strongly determined by the kinetic parameters in the combustion rate expressions. By modifying the homogeneous gas phase combustion rates by constant factors such that

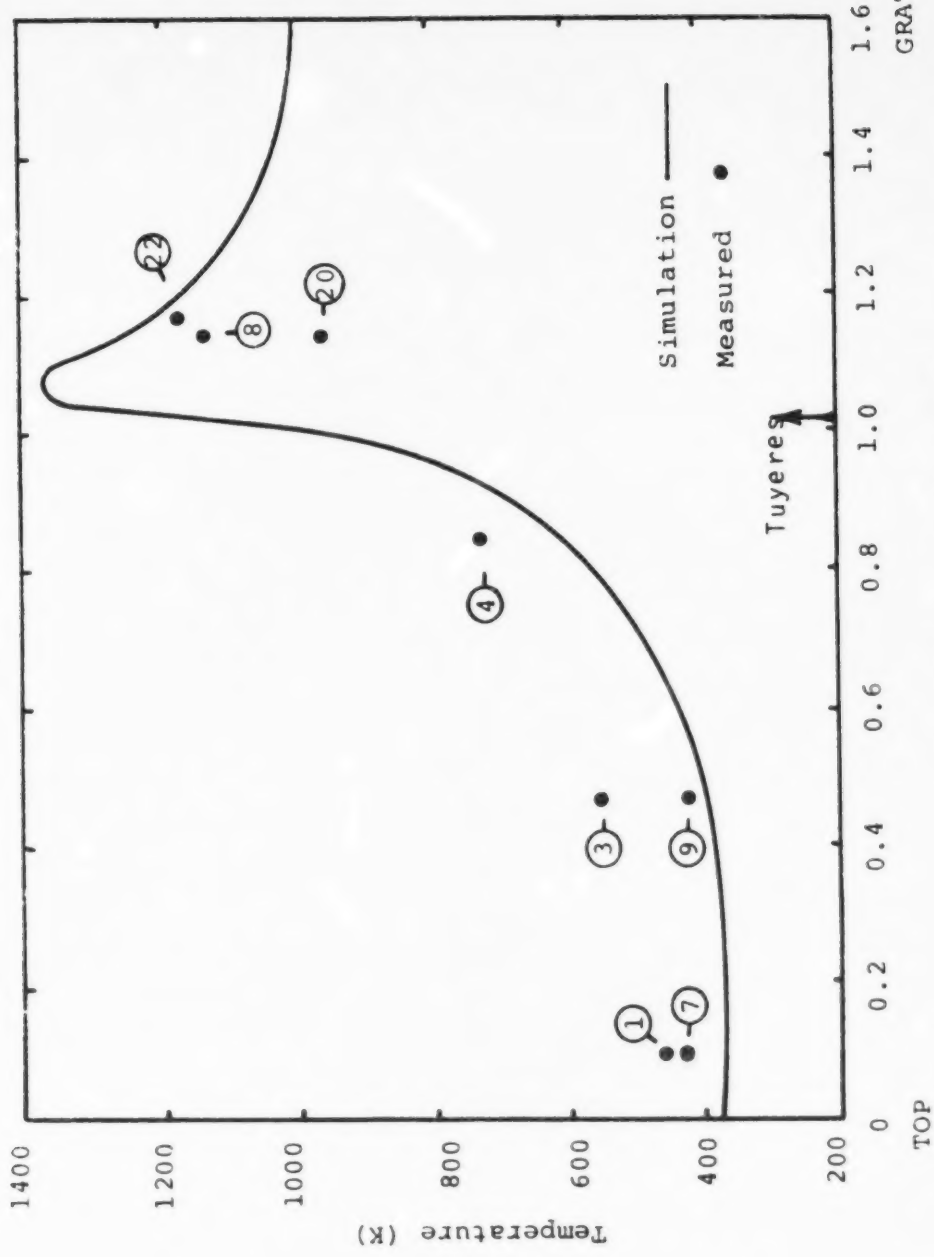

Figure 13 : Expected Temperature Profile

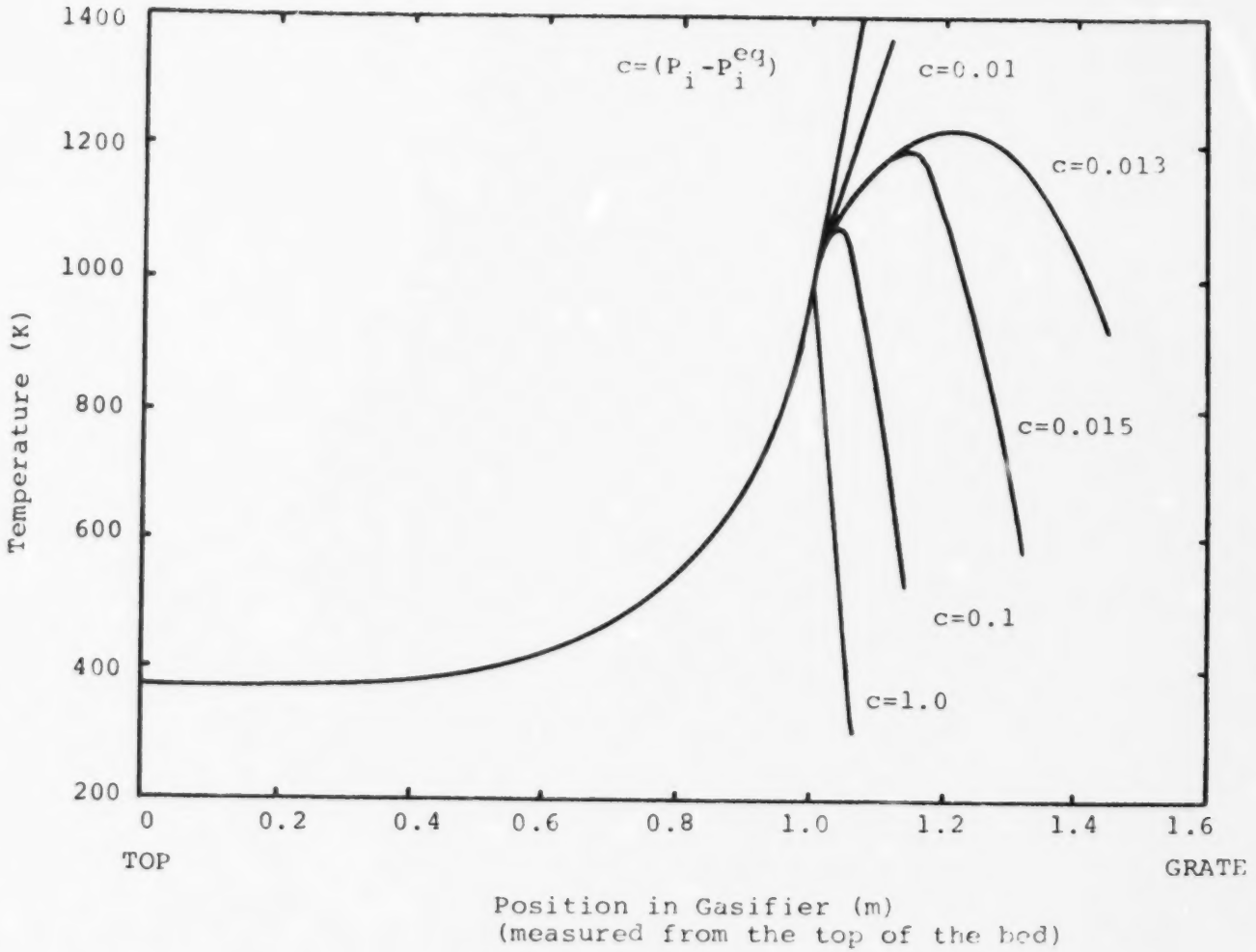

Figure 14 : Simulated Temperature Profile with Modified Combustion Rates

Modified R_i = c(original R_i) where c = 1.0, 0.1, ... etc.

the temperature profile changes radically (Figure 14). When introducing these modifications it is possible to shift the location of the maximum temperature to a point nearer the end of the combustion zone. However, after reaching the maximum the temperature still drops monotonically to zero (except if c is very small, in which case the temperature does not reach a maximum but rises monotonically).

Since the cause of the unexpected behaviour of our predicted results has not been isolated, further analysis of the combustion and gasification models has not been attempted.

2.7.3.1 Problems with the Combustion Model

When considering the difficulties which were encountered in the combustion region the methods used to incorporate the air distribution model were scrutinized. Two approaches had been considered. In one, the air was distributed on a differential scale, while in the other it was distributed on a finite scale.

The finite scale air distribution model was introduced to the simulation in the MAIN program. There, a fraction of the total air feedrate was added to the local compartment (Δz) according to both the air distribution function and the location of the compartment with respect to the tuyere level. So, for the purpose of calculation, the compartment saw an instantaneous injection of mass at z. The numerical package DGEAR is unaware of this injection except through the information provided by a flag called INDEX. If changes are introduced to the independent variables outside of DGEAR then INDEX must be set to 1 so that the changes will be recognized. However, by setting INDEX to 1 all previous

information about the independent variables is lost to DGEAR.

A problem is encountered here. The numerical package DGEAR is a backward differentiation technique, i.e. it uses previous information to predict the next value of the independent variable. When we introduce an instantaneous injection of mass on a finite scale, the discontinuity which results renders all previous information unsuitable for future predictions. DGEAR restarts its calculation at z using the most recent value of the independent variable as a new initial value. Thus, the advantages of backward differentiation are lost in the combustion region if this approach is taken.

The alternative, a differential scale air distribution model, was introduced to the simulation in the combustion section of the FCN subroutine. There it was incorporated in the differential equations directly. In this case, there is again an instantaneous injection of mass. However, now it is occurring on a differential scale and the numerical package DGEAR is aware of the change intrinsically. Previous information about the independent variables is still valid for prediction and the advantages of the backward differentiation technique are still available for the solution of the mass and energy balances in the combustion region.

The differential scale distribution model appears to be the route to take. However, we had difficulty in getting the oxygen balance to close when this technique was used. Oxygen and nitrogen balances are intimately related within the combustion zone since the sum of their mass flowrates is equal to the total air feedrate. Yet, although the nitrogen balance behaved well, the oxygen balance did not. At a point below the tuyere level where all of the air has

already been introduced to the gasifier, the net oxygen flowrate (including gaseous oxygen and elemental oxygen associated with water, carbon monoxide and carbon dioxide) was about twice the value that it should have been, even when the elemental oxygen contribution from the wood and moisture was considered.

In attempting to locate the source of this oxygen balance error, we considered the fundamental formulation of the problem. Of the eleven differential equations in the simulation, nine represent the mass balances of the individual species which exist in the gasifier (char, water, hydrogen, methane, carbon monoxide, carbon dioxide, oxygen, nitrogen and wood). As expected, the changes in the flowrates of these species are interrelated by other balances, namely the overall mass balance and the element balances for carbon, hydrogen, oxygen and nitrogen. Since these other balances are invoked indirectly via the stoichiometry of the reactions, the nine differential equations are not all independent.

When the equations are not all independent, numerical problems can be encountered. It is possible that a singular inversion matrix is being created by DGEAR. The presence of singularities or near singularities may introduce a significant error to the predictions of the independent variables and this may be the reason for the unexpected behaviour that was noted in Figure 12. Before further development of the model or the simulation is attempted, the differential equations should be reduced to an independent set. The excluded independent variables can be calculated subsequent to the solution of the differential equations by invoking the mass and element balances.

A number of parameters are used by DGEAR to control the solution of the differential equations. These parameters

(METH, MITER, H, TOL) are set at suitable values for executing version 83-09 of QUGAS2. However, if changes are made to the simulation (such as the suggested reduction of the differential equations to an independent set) then perhaps new values of these parameters will be more appropriate.

A final consideration in resolving the problems which were encountered with version 83-09 is the selection of a different numerical technique. In particular, the second derivative formulas used in SECDER [50] might be examined for application in this down-draft wood gasifier simulation.

2.7.4 Conclusions About the Simulation

The models for the drying and pyrolysis zones produce reasonable predictions of the extent of these regions in the down-draft wood gasifier, as determined by comparison with experimental observations made by Saskatchewan Power, Groeneveld and SERI. The appropriateness of the pyrolytic product distribution, however, will remain unknown until experimental data in the form of gas sample compostions from interior points of the gasifier become available.

Numerical problems encountered in the simulation of the combustion model have yet to be resolved. A number of approaches have been suggested for solving these problems.

Due to the difficulties encountered in the combustion section of the simulation, the model has not been fully evaluated. Both the gasification and post-reaction sections are untested since the sequential computation never reached these regions of the gasifier. Therefore, before the 83-09 version of QUGAS2 can be used, further examination of these parts of both the model and the simulation must be

performed.

3. EMPIRICAL MODELLING OF DOWN-DRAFT GASIFIER OPERATION

3.1 Empirical Models of the Saskatchewan Power Gasifier Operation

From July to October 1982, the Saskatchewan Power Corporation Research Centre (SPC) conducted experiments on their Imbert down-draft gasifier according to an experimental design provided by the authors of this report. A 5-variable, 32-run central composite design was prepared (Table 7) to study the individual and joint effects of the following variables:

i) wood particle size (cm) (S)
ii) wood moisture content (wt% wet basis) (M)
iii) electrical load (kW) (L)
iv) air preheat temperature (°C) (P)
v) grate bumping rate (agitations per hour) (G)

Five measures of gasifier performance were selected:

i) gas production rate (m^3/min at 288K, 1 atm) (GAS RATE)
ii) gas temperature at the exit from the gasifier (°C) (GAS TEMP)
iii) maximum temperature in the gasifier (°C) (MAX TEMP)
iv) higher heating value of the gas produced (MJ/m^3 dry gas) (HHV)
v) volumetric ratio of carbon monoxide to hydrogen (CO/H2)

In the selected experimental design each variable is examined at five levels, making it possible to fit a full quadratic model to the data. However, due to a number of factors, notably poor carbon balances and equipment

Table 7: Experimental Design for the SPC Experimental Program

Run #	Wood Size (in grain direction) (mm)	Moisture (wet basis)	Electrical Load (kW)	Air Temp. (°C)	Grate Frequency
1	25	15	30	125	4
2	38	10	25	75	5
3			25	175	3
4			35	75	3
5			35	175	5
6		20	25	75	3
7			25	175	5
8			35	75	5
9			35	175	3
10	52	5	30	125	4
11		15	20	125	4
12			30	25	4
13			30	125	2
14			30	125	4
15			30	125	4
16			30	125	4
17			30	125	4
18			30	125	4
19			30	125	4
20			30	225	4
21			30	125	6
22			40	125	4
23		25	30	125	4
24	64	10	25	75	3
25			25	175	5
26			35	75	5
27			35	175	3
28		20	25	75	5
29			25	175	3
30			35	75	3
31			35	175	5
32	89	15	30	125	4

failures, the usable data set contained only 15 runs (Appendix A.4). With this reduced data set, the fitting of individual terms in the full quadratic model was examined by a forward stepwise regression technique. Recognizing that the precision of the resulting fitted models is considerably less than would have been possible with the full 32 designed runs, the following empirical models have been found to represent the data best. The right hand column in the following summaries shows values of the multiple correlation coefficient R^2 (a value of 1.0 would indicate a perfect fit of the model to the data). Comparisons of the fitted models with the experimental data are shown in Figure 15. Each model is statistically adequate, and none shows any lack of fit. However, it should be noted that there is a considerable scatter in the data. Three significant figures are reported for each coefficient for maximum computational precision. This number of significant figures does not represent, however, the accuracy of the model fit.

	R^2
GAS RATE = - 6.07 E-2 + 1.33 E-1 (L) - 6.61 E-3 (P) - 1.55 E-3 $(L)^2$ + 3.69 E-5 $(P)^2$	0.85
GAS TEMP = 4.31 E2 + 6.51 E-3 (S)(P)	0.65
MAX TEMP = 9.95 E2 - 2.09 E-1 (P)(G)	0.56
HHV = 5.16 - 4.36 E-3 (P)	0.37
CO/H2 = 1.06	----

It should be noted that there are high correlations between all terms involving the preheat temperature (P), and between all first and second order terms which involve the same

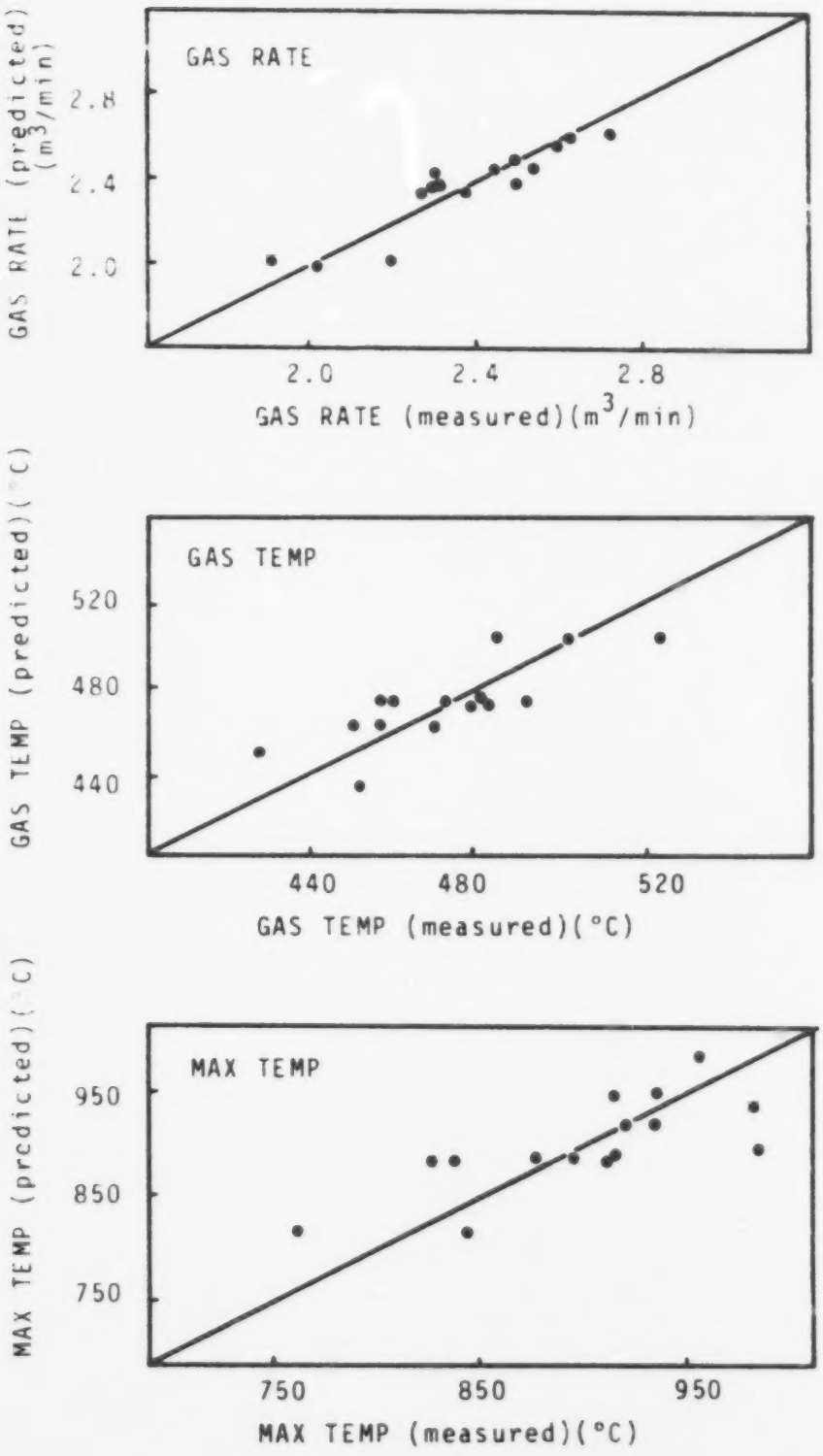

Figure 15 : The Empirical Models:
Predicted vs Measured Values of the
Performance Measures

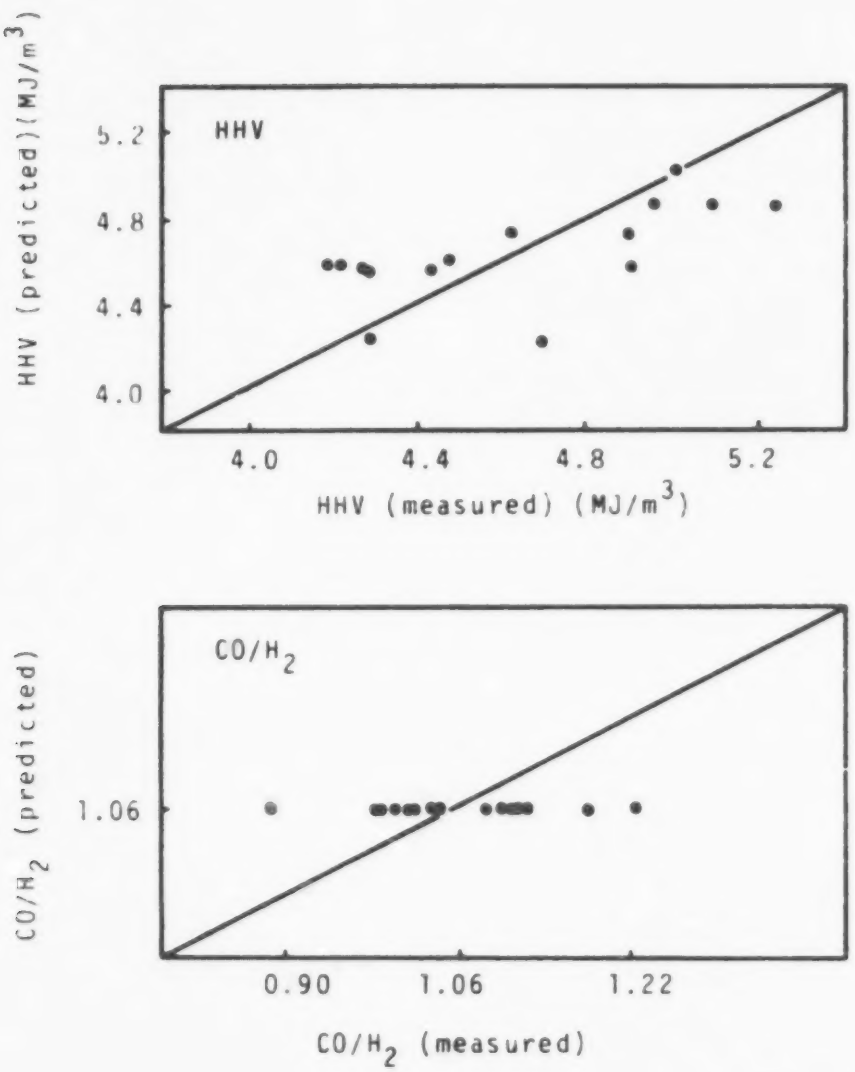

Figure 15 (cont'd) : The Empirical Models:
Predicted vs Measured Values
of the Performance Measures

variables (e.g. L and L^2). When P is substituted for the cross-product terms (S)(P) and (P)(G) in the fitted models for gas temperature and maximum temperature, and $(L)^2$ is eliminated from the model for the gas production rate, the resulting models are still statistically adequate; however they account for a smaller fraction of the variation in the data, as shown by the smaller R^2 values.

	R^2
GAS RATE = 1.56 + 2.04 E-2 (L) + 1.38 E-3 (P)	0.45
GAS TEMP = 4.32 E2 + 3.40 E-1 (P)	0.50
MAX TEMP = 9.98 E2 - 8.15 E-1 (P)	0.44

The preheated air temperature appears to be an important factor in all of the measures of performance, as is expected. However, the negative coefficients for the terms involving this variable in the models for the maximum temperature and higher heating value are not expected.

The electrical load, which controls the air feedrate for a suction-type gasifier such as the Imbert, is expected to be of importance in the gas production rate and this is confirmed in the GAS RATE model.

The absence of the influences of wood particle size, wood moisture content and grate agitation rate is not surprising. It appears that there is a broad range of each of these variables over which it is possible to operate with similar results. Only when attempting to operate outside of these ranges would these variables be expected to affect gasifier performance. For example, it is widely reported that gasifiers can handle a wide variety of feedstocks.

Generally, feedstocks with moisture contents of less than 50wt% can be processed. This upper limit is imposed by the constraint of thermal sufficiency. Above this limit, it is necessary to include an external energy source (e.g. wood dryer) to maintain operation of the gasifier. Similarly, a wide variety of feedstock particle sizes can be processed easily. A lower limit on size is imposed by a requirement that the pressure drop across the bed be low enough that air and gas can flow through the bed. (An upper limit is imposed by the physical dimensions of the gasifier.) Finally, the only purpose of grate agitation, it appears, is to control the pressure drop across the bed by periodically knocking loose the ash which collects in the lower part of the gasifier.

3.2 Comparison with Forintek Results

The Forintek laboratories have also examined the operational behaviour of the down-draft wood gasifier. Their gasifier is similar to the SPC Imbert unit, the only major differences between the two being that the Forintek unit has a concentric, flat choke-plate rather than a conical restriction to flow in the vicinity of the tuyeres and air is forced in through the tuyeres with a blower rather than drawn in by downstream suction.

The results in Section 3.1 appear to be different from those found by Forintek [35]. They report the following correlation:

GRATE TEMP = 928.93 + 169.56 S + 42.9 G - 1.55 M

where	GRATE TEMP	is the grate temperature (°F)
	S	is the average chip size (inches)
	G	is the grate rotation rate (rev/hr)
	M	is the moisture content (wt%)

The Forintek grate temperature was expected to show behaviour similar to that of the SPC maximum temperature. (The SPC maximum temperature is the maximum of the recorded temperatures in their Imbert gasifier. This may not correspond with the actual maximum temperature in the gasifier which may exist at a point where there is no thermocouple for measurement. The temperature measurements which were used in the MAX TEMP regression of the SPC data were those taken closest to the grate. The distance between these measurements and the grate is estimated to be 20 cm.) Yet, whereas the regression of the SPC data indicated that wood particle size, grate agitation and wood moisture content have insignificant effects on the maximum temperature (MAX TEMP), Forintek's regression includes all of these terms.

In attempting to analyze this disagreement, it was noted that Forintek's experimental work was conducted in a different range of wood particle size, 5 to 50 mm. This particle size range may extend below the lower limit mentioned earlier, where pressure drop becomes a significant factor.

The grate designs are very different in the Forintek and Saskatchewan Power gasifiers, being a continuous rotating mechanism in the former and a periodic agitating device in the latter. It is difficult, therefore, to compare their effects quantitatively. The significance of this effect in the Forintek results suggests that the rotation rate in that study may have been too fast, with the result that char was removed before being completely consumed by the gasification reactions. Indeed, Forintek records higher char and ash yields (2.5-7% of total mass input) than does Saskatchewan Power (0.2-0.3%). This may mean that in the Forintek study the char at grate level had a high carbon content and that the gas-solid reactions were progressing still. This would

account for the positive effect of the grate rotation rate on grate temperature: the faster the rotation, the faster the char is removed from the gasifier, the higher the carbon content of the char being removed, and the more significant the gas-solid reactions at grate level.

In the Forintek study the moisture content was controlled at levels (7% to 26%) similar to those in this study (10% to 25%), and therefore would be expected to have a similar effect on product temperature. However, the presence of a moisture content effect in the Forintek results and the absence of it in the Saskatchewan Power results is an inconsistency for which an explanation is not obvious, aside from the possible effects of correlations among the variables in the empirical models due to the incomplete data set.

The SPC MAX TEMP regression indicated that this temperature is significantly affected by the preheated air temperature. Forintek's regression does not show this effect because air temperature was not a variable in their investigation.

Due to the difficulties encountered in the simulation of the mechanistic model we do not have simulated results (for the gas production rate, the final gas temperature, the maximum temperature, the higher heating value and the carbon monoxide to hydrogen ratio of the product gas) to compare with the SPC data. However, when these problems are solved the SPC data set will be useful for evaluation of the model.

4. THE COLLECTION AND ANALYSIS OF GASIFIER OPERATING DATA

The final area to be addressed in this report is that of the reliability and acceptability of data from gasifier operation. The type of data collected often differs between projects. However, there are general issues involved in specifying and determining the acceptability of data, and in coping with typical problems which occur in industrial or pilot-plant scale data collection. Some of these problems were discussed in the previous section on empirical modelling using the SPC data. We will now use the SPC data collection as a basis for reviewing state-of-the-art techniques for coping with typical problems in data collection.

4.1 The SPC Data Set

Saskatchewan Power Corp. provided data (Figure 17 and Table 14 - Appendix A.4) from start-up to shut-down for each run, a period of from 4 to 5 hours. In order to identify the steady state values for each measured variable, the data were plotted against time and steady state periods were chosen visually from the plots. Estimates of the arithmetic mean and standard deviation were then computed using the data within the selected steady state period for each variable. These values (Table 15 - Appendix A.4) were used in fitting the empirical models for gasifier operation (Section 3).

4.2 The Mass Balance: A Measure of Data Reliability

In the experimental design that we supplied for SPC, we indicated that a mass balance should be performed following each run so that the acceptability of the run could be determined immediately. Limits of $\pm$ 10% for the mass

balance were set and accepted by SPC. The computed mass balance for each run is shown in Table 8.

Figure 16 is a schematic representation of the SPC process, indicating the nature and location of measurements. In our recommendations for the work to be performed under ENFOR contract C-197a we specified a "complete" set of experimental measurements. Each of the measurements in this set is essential if the overall mass balance is to be used as an indicator of run acceptability. In the absence of some of these measurements, process constraints (e.g. element balances) must be used to compute values for the missing measurements. Those balances, then, cannot be used to measure the acceptability of the experimental runs. In the SPC data set the air feed rate and raw product gas moisture content were not measured. As a result, hydrogen and nitrogen element balances were necessarily invoked in the overall mass balance calculation. Consequently, for the SPC data set the overall mass balance for an experimental run was expected to be a poor indicator of the acceptability of that run.

The carbon element balance, however, remained a useful measure of acceptability, being independent of the computed values for air feed rate and product gas moisture content. The carbon balance and overall mass balance for each run are summarized in Table 8. Deviation from the mass balance limits of $\pm$ 10% is more obvious for the carbon balance and several runs were deemed unacceptable on this basis. Only the runs for which the carbon balance error was less than $\pm$ 10% were used in fitting the empirical models.

The difficulties that we encountered with the SPC data are not uncommon in dealing with an experimental study on large scale equipment. In the following section we outline a general statistical approach for analyzing data in such situations.

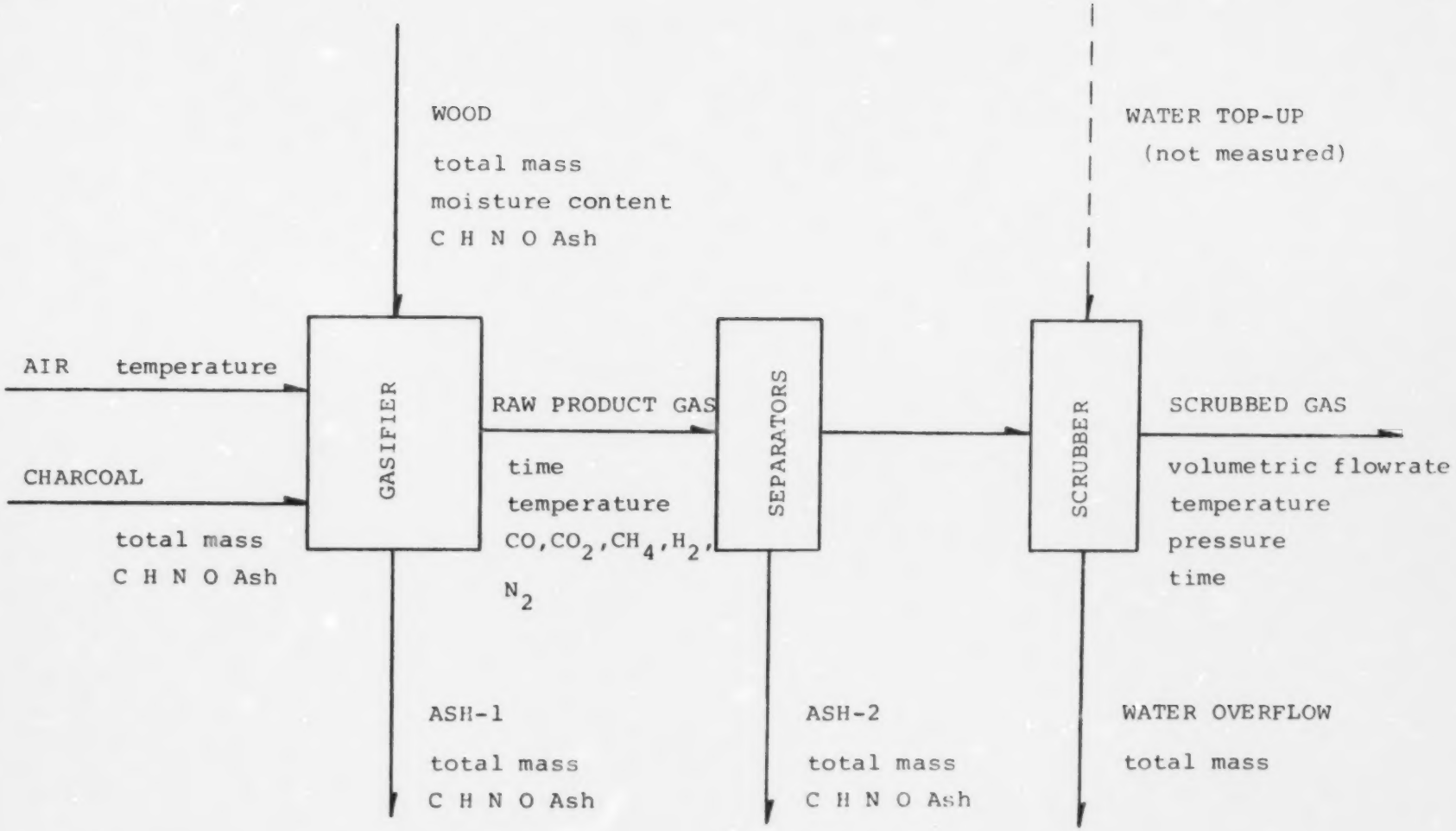

Figure 16: Saskatchewan Power Corp. Gasifier Flowsheet (including measurements)

Table 8. Overall Mass Balances and Carbon Balances (SPC)
(Mass Out/Mass In)

Run #	Overall Balance	Carbon Balance	
R8	-	-	
R10	-	-	
R11	-	-	
R12	1.00	1.02	
R13	1.01	1.10	
R14	0.98	0.83	*
R15	1.00	1.03	
R16	1.01	0.99	
R17	1.00	0.93	
R19	0.96	0.80	*
R21	-	-	
R22	0.99	1.01	
R23	1.00	1.10	
R24	0.98	0.90	
R25	1.00	0.99	
R26	0.96	0.79	*
R28	1.02	1.14	*
R29	0.95	0.90	
R30	0.98	0.95	
R31	1.01	1.13	*
R32	1.04	1.13	*
R34	0.97	0.84	*
R35	0.96	0.84	*
R37	1.01	1.03	
R38	1.01	1.03	
R39	1.02	1.06	
R40	1.00	0.97	
R41	1.02	1.08	
R42	0.98	0.83	*
R43	1.04	1.07	
R44	1.00	0.99	

* exceeds mass balance limits of ± 10%
\- cannot be computed using this technique
(no GC analysis available)

4.3 Statistical Analysis of Constrained Data Sets

Three main problems are encountered in attempting to use experimental data to analyze the performance of a unit or process.

First, all measurements are subject to errors which make the data set inconsistent with system constraints such as material and energy balances. Measurement errors can be of two types: random errors which are usually assumed to be independent and normally distributed with zero mean, and gross errors which are caused by non-random events such as instrument biases, instrument malfunctioning or process upsets. Incompatible data can also arise from incomplete or inaccurate process models.

Secondly, the data set is usually incomplete. Some process variables may not be measured for reasons that include convenience, cost and technical feasibility.

Thirdly, there is usually a profusion of data available, especially for processes which are automatically monitored and controlled. The available data may be both spatially and temporally redundant. Such quantities of data will usually be more than would be necessary to analyze system performance if the measurements were not subject to errors. Is averaging over time an appropriate technique for producing a representative set of measured data? Stanley and Mah [36] have successfully applied the discrete Kalman filter to a process network with both spatial and temporal redundancies in the data. "By adjusting the relative weights of process noise and measurement noise covariances the filter could be tuned to give significant error reduction"(error in mass and energy balances). They also note that "the redundant measurements contributed significantly to the overall error reduction".

Each of these problems is encountered in attempting to analyze the SPC data and several questions arise. How can the data be adjusted to satisfy the process constraints? How can unmeasured variables be estimated from the measured data set? How can gross errors be detected and identified? What are the most efficient locations for measurements in a process? The final question has only been addressed recently [37] and no entirely satisfactory solution has been proposed yet. The first three questions have received considerable attention in the literature, with many of the basic concepts being repeatedly rediscovered. Knepper and Gorman [38] have addressed the problems of data reconciliation and the detection of gross errors,and their algorithm is also useful in estimating unmeasured variables. Their work is state-of-the-art and is summarized here.

4.3.1 The Data Adjustment Algorithm

The data adjustment algorithm proposed by Knepper and Gorman is similar to earlier algorithms [39,40] in that it is based on least squares analysis and assumes that the data set is subject to random, independent, normally distributed errors only.

The data adjustment problem requires that values of the process variables Z be adjusted to provide estimates $\hat{Z}$ which satisfy a set of constraints $F(\hat{Z})=0$. Knepper and Gorman have generalized the problem to a case in which parameters θ as well as adjusted data may be estimated, $F(\hat{Z},\hat{\theta})=0$. However, the measured data will not usually satisfy the process constraints with the result that

$$F(Z_o,\theta_o) = G_o \neq 0 \qquad (1)^*$$

---

*The nomenclature used in Sections 4.3 to 4.3.6 is described herein. These symbols should not be confused with those used in previous sections.

where Z_o and θ_o are the measured data set and initial estimates of the parameters, respectively, and G_o is the departure from satisfaction of the constraints. To accommodate nonlinear constraints equation (1) can be expanded using a first order Taylor series approximation about the initial values of Z_o and θ_o, and the result projected to the solution $F(Z_i, \theta_i)=0$. This leads to an iterative solution:

$$F_z(Z_{i+1}-Z_i) + F_\theta(\theta_{i+1}-\theta_i) = - G_i, \quad i=0,1,... \qquad (2)$$

where F_z and F_θ denote partial derivatives of F with respect to Z and θ.

However, since it is the total adjustment that is to be minimized it is more appropriate to examine $(Z_{i+1} - Z_o)$. Equation (2) is therefore more usefully expressed in the form

$$F_z(Z_{i+1}-Z_o) + F_\theta(\theta_{i+1}-\theta_i) = - G_i + F_z(Z_i-Z_o) \qquad (3)$$

Since some measurements will be considered to be more precise than others, the required adjustments are weighted by the inverse of the variance-covariance matrix of the measured data, $R=[\sigma_{i,j}]$, which is usually estimated by the diagonal matrix formed by the sample variances for the measured variables. The constraint discrepancies, G, are also normalized, in this case by the variances of the discrepancies due to measurement error, $(F_z R F_z^T)$. Knepper and Gorman then define a new set of vectors which are used to simplify the presentation of the solution. Defining

$$d_{i+1} = D\,(Z_{i+1}-Z_o)$$

$$g_i = H\,G_i$$

$$D^T D = R^{-1}$$

$$H^T H = (F_z \, R \, F_z^T)^{-1}$$

and substituting for Z and F in equation (3) and multiplying through by H, the result is

$$H \, F_z D^{-1} d_{i+1} + H \, F_\theta (\theta_{i+1} - \theta_i) = -g_i + H \, F_z D^{-1} d_i \qquad (4)$$

Notice that $d_i^T d_i$ is equivalent to $(Z_{i+1} - Z_o)^T \, R^{-1} (Z_{i+1} - Z_o)$. Minimization of this objective function will give the least squares estimates of the required data adjustments.

Knepper and Gorman suggest a two-stage solution to this problem. First the parameters are estimated to minimize the portion of the objective function which does not involve the measured variable adjustment,

$$\min \left\| -g_i + HF_z D^{-1} d_i - HF_\theta (\theta_{i+1} - \theta_i) \right\| \qquad (5)$$

giving a least squares fit for G_o. Then the weighted least squares adjustment of the measured data is calculated,

$$\min \left\| d_{i+1} \right\| \qquad (6)$$

Now Knepper and Gorman invoke the theory of generalized inverses to solve equation (4). Defining $Q = (F_z R F_z^T)^{-1}$, and rewriting in terms of the original variables, they obtain

$$\theta_{i+1} - \theta_i = (F_\theta^T Q F_\theta)^{-1} \, F_\theta^T Q \, [-G_i + F_z (Z_i - Z_o)] \qquad (7)$$

for estimates of the parameters, and

$$Z_{i+1} - Z_o = R F_z^T \, Q [I - F_\theta \, (F_\theta^T Q F_\theta)^{-1} F_\theta^T Q \quad] [-G_i + F_z (Z_i - Z_o)] \qquad (8)$$

for the required data adjustment. As they clearly state, this problem can only be solved if the constraints are independent and usefulness of the predicted adjustments is entirely dependent on the appropriateness of both the specified variance-covariance matrix and the process model.

The authors have recognized that similar equations have been developed by other investigators (Ripps, Nogita and others) using the method of Lagrange multipliers. The contribution of Knepper and Gorman has been in generalizing the solution to accommodate models with nonlinear constraints and models requiring parameter estimation. They also claim that the method of generalized inverses provides more insight to the form of the solution although we are not convinced that this is the case.

4.3.2 Computational Aspects of the Adjustment Algorithm

"Problems of practical interest can easily reach a size such that the solution of equations (7) and (8) requires a significant amount of computing time "[38]. To reduce the required computing time Knepper and Gorman propose a "constant direction" algorithm:

1) Evaluate θ_o by some technique (such as rough guesses or by solving a set of only p of the constraints) and set Z_o = measured values.

2) Evaluate the partial derivatives F_z and F_θ at θ_o and Z_o. (The bulk of the matrix transposition, inversion and multiplication is done in this step.) Compute

$$E' = RF_z^T Q(I - F_\theta B')$$

$$B' = (F_\theta^T Q F_\theta)^{-1} F_\theta^T Q$$

$$E = E'F_z$$

$$B = B'F_z$$

3) Evaluate successive estimates Z_i and θ_i using the following simplified forms of equations (7) and (8) until convergence is achieved, i.e. until $F(Z,\theta)=0$.

$$\theta_{i+1} - \theta_i = -B'G_i + B(Z_i - Z_o)$$

$$Z_{i+1} - Z_o = -E'G_i + E(Z_i - Z_o)$$

These relations can be further simplified to give

$$\theta_{i+1} - \theta_i = -B'G_k$$

$$Z_{i+1} - Z_i = -E'G_k$$

where $G_k = \sum_1 G_i$

4) Set $\hat{\theta} = \theta_1$ and $\hat{Z} = Z_1$ Check the value of d^Td. If there is little change from the preceding iteration then the calculations are complete. Otherwise return to step 2.

Because of the effort required in step 2, restriction to periodic updating of B' and E' after local convergence should result in reduced computing time. However, the authors note that the stability of this algorithm has not been tested. If stability is a problem they suggest a modified Gauss-type of approach where the adjustments ($Z_{i+1} - Z_i$) can be moderated by a scalar quantity between zero and unity.

The convergence criterion that they suggest requires that the change in the weighted sum of squares of adjustments not change significantly between successive iterations. Bates and Watts [41] have shown that this can be a poor indicator of true convergence, especially if the solution surface is relatively flat. The amount of effort required to obtain adjusted estimates of the variables may be sufficient justification for implementing a more appropriate convergence criterion.

4.3.3 Generality of the Solution

Is this solution going to be useful in adjusting any set of data? No, unfortunately not. There are some potential problems that it will not be able to handle. Some limitations are more serious than others.

In many processes only selected "streams" are monitored. When some streams are not measured a node-aggregation scheme can be implemented to provide a solution in the absence of the intermediate data. This is the popular "control volume" approach in which only streams crossing the "control boundary" are necessary in computing a material or energy balance. Therefore selected stream monitoring will not be a potential problem for the Knepper-Gorman data adjustment algorithm.

However, in some cases not only are all streams not monitored but for those streams which are monitored a full set of data is often not collected, e.g. temperatures are measured but flow rates are not, or vice versa. This problem is encountered in the SPC data set where measurements of the moisture content of the raw product gas and air flow rate are missing. Knepper and Gorman make no comment on how to deal with such a situation. At first glance it does not appear that the algorithm can accommodate a situation in which an incompletely measured stream cannot be eliminated by the node aggregation method. However, if the missing measurements are delegated to the status of parameters then they can be estimated. This is one major advantage of the Knepper and Gorman extension to include the estimation of parameters. Incomplete measurement is more the rule than exception in the process industries.

Another potential problem is encountered in interpreting the

adjusted data set if the constraints are not written in terms of the primary measured variables (typically pressure, temperature etc.) but rather in terms of derived variables which are often nonlinear functions of the primary variables (e.g. mass flowrates, enthalpies etc.). The problem lies in the specification of the variance-covariance matrix of the "measured" quantities and in linearization of the objective function since first order expansion of a function is a reliable representation only in the case of a model which is nearly linear in the required adjustments.

Finally, the least squares data adjustment technique is only statistically acceptable if there are no gross errors in the data set. Because of the nature of the least squares computation, the effect of a gross error can affect the full set of adjustments. In such a case, not only will the source of the gross error be obscured but the computed adjustments for all variables will be incorrect, possibly leading to misinterpretation of process performance. No data adjustment algorithm based on the assumption of normally distributed errors can account for gross errors. Therefore it is necessary to eliminate the gross errors from the data set before data adjustment is attempted. Knepper and Gorman have considered this problem.

4.3.4 Detection of Gross Errors

Two problems are associated with the presence of gross errors: detection and isolation. Ripps [40] was the first to publish a technique for identifying and discarding measurements as gross errors. His procedure requires the data to be segregated a priori into those suspected to be subject to random error alone and those suspected to be subject to gross errors. This requires operator experience which indeed is often the most efficient way to locate process problems. Ripps advocated discarding one measure-

ment at a time and comparing the sums of squares of the required data adjustments with and without that measurement. One limitation in the Ripps procedure is that it contains no criterion which specifies when enough data have been discarded to assert, with some confidence, that the remaining data are subject to random errors alone. Another major limitation is that the detection of gross errors is attempted only after the data adjustment has been performed. As mentioned before, data adjustment may often be insensitive to the presence of gross errors and may make them difficult to isolate because of the smearing effect of the least squares adjustment.

Nogita [39] introduced a statistical test of data inconsistency using a test function A, where

$$A = \sum_i \frac{(Z_{i+1} - Z_o)}{\sigma_i} \qquad (9)$$

If A is a linear function of the measurements Z, and the Z are normally distributed, then A is also normally distributed with variance σ_z. A normalized version of A, denoted by N where

$$N = A / \sigma_z \qquad (10)$$

is then compared with the unit normal distribution at a selected significance level α. For instance, for $\alpha = 0.1$ a gross error is suspected when $|N| > 1.645$. Nogita proposed a serial elimination algorithm similar to that of Ripps in which one measurement at a time is discarded and replaced. In this case the values of $|N|$ are compared to determine which measurements are to be discarded permanently. This test also requires that the data adjustment be performed first. Another point of interest is that Nogita's test uses linear combinations of all the residuals and therefore it is possible for gross errors to pass unnoticed because of error

cancellations.

Mah et al [42] seem to have been the first investigators to recognize the necessity of early detection of gross errors. In a development similar to Nogita's they defined a test function A' which again is compared with the normal distribution, where

$$A' = H^{-1} F_m Z_o \tag{11}$$

and $$H_{i,j} = \begin{cases} (F_m R_d F_m^T)^{1/2}_{ij} & , i=j \\ 0 & , i \neq j \end{cases}$$

The advantage of this test function is that it can be applied before the data reconciliation, and as a result it is more sensitive and takes less time to compute. Secondly, while Nogita used a single test statistic for the entire process this test function provides a separate test statistic for each node in the process.

Knepper and Gorman do not appear to have been aware of the above formulation for they introduce another multivariate test statistic:

$$A'' = F(Z_o, \theta_1)^T (F_z R F_z^T)^{-1} F(Z_o, \theta_1) \tag{12}$$

which, when compared with a χ^2 distribution with (m-p) degrees of freedom, should reveal the presence of gross errors in the data set. Again the test procedure involves sequential elimination and replacement of each measurement, with the A" test determining each elimination. Knepper and Gorman suggest that this test be used to isolate those measurements having gross errors and that the corresponding quantities be treated as parameters to be estimated. In

such cases the test should be repeated with a reduced number of degrees of freedom. As the authors have noted, there is no statistical basis for eliminating more than one measurement at a time. Therefore, if the A" test reveals two suspect measurements some other criterion must be used to discriminate between them. Furthermore, they note that although the A" test is more sensitive than other available tests, it will still fail to reveal even relatively large gross errors in some cases. "The problem of detecting errors becomes more difficult as the ratio of data items to the number of constraints minus parameters increases "[38].

It should be noted that if the data fail this test it may be due to the presence of gross errors, to inappropriate assignment of measurement variances, or to an inappropriate model. A data set can still be estimated which will satisfy the process constraints; however, unreasonably large variances will be associated with the model predictions.

Notice also that if data are discarded because they are suspected of being in gross error then replicate runs in the data set are essential at those conditions. Otherwise, the node aggregation method must be used, if applicable, or the measurements must be relegated to the status of parameters to be estimated.

4.3.5 Error Structure of the Adjusted Data

Using a method outlined by Britt and Leucke [43] Knepper and Gorman also develop expressions for the variance-covariance matrices for the estimated parameters and the adjusted process variables. These expressions are

$$(F_\theta{}^T Q F_\theta)^{-1} \qquad (13)$$

for the parameter estimates and

$$RF_z^T QF_z R - RF_z^T QF_\theta (F_\theta^T QF_\theta)^{-1} F_\theta^T QF_z R \qquad (14)$$

for the adjusted variables.

They suggest two uses for this information. First, by comparing the size of the required data adjustment $(\hat{Z}-Z_o)$ with the estimated standard deviation of the adjustment, a χ^2 test can be used to detect gross errors. This method is not as useful as the other method proposed by Knepper and Gorman since, again, it requires that the data adjustment be performed first . Secondly, they propose that the variances of these adjusted data be used to assess the value of obtaining additional measurements to enhance the precision of the adjusted data set.

4.3.6 Conclusions About Data Adjustment

Knepper and Gorman have addressed a number of important data analysis problems, including data adjustment to satisfy process constraints, estimation of parameters and unmeasured variables, detection and isolation of gross errors in the data set and determination of the value of additional measurements. Each of these problems is commonly encountered when analyzing experimental data.

However, there remains one fundamental limitation in their technique - adjustment of the data requires knowledge of the variance-covariance matrix for the measurements. Because it is unlikely in most situations that appropriate data will be available for estimation of covariances, the covariances will often be assumed to be negligible and a diagonal variance-covariance matrix used instead. Yet estimation of the variances of the measurements requires replicate ex-

periments and even this information is often not available.

Recently these techniques were applied to the Saskatchewan Power Corp. data set [44]. The Knepper and Gorman data adjustment algorithm proved to be very efficient - convergence was achieved in two or three iterations. However, as was noted above, the success of the algorithm was found to be dependent on the variance-covariance matrix. Beginning with a set of initial estimates of the measurement errors which we provided, Perriott was able to refine the set to one which yielded acceptable results. However, even then a number of measurements were found to be suffering from gross errors. Copies of this report are available from Queen's University.

NOMENCLATURE

$A, A^{\circ}A'$	statistical test functions used in detecting gross errors (in section 4.3 to 4.3.6)
A'	cross sectional area of gasifier in direction of flow
A_o	outer surface area of gasifier wall for radial heat transfer
A_i	inner surface area of gasifier wall for radial heat transfer
A_{lm}	log mean of A_o and A_i
C_{pl}	heat capacity of species i
d_e	effective diameter
d_p	particle diameter
d_t	gasifier bed diameter
d_1	diameter of outer surface of inner wall of gasifier
d_2	diameter of inner surface of outer wall of gasifier
D	diffusivity
D_e	effective diffusivity
e_i	mass fraction of species i in pyrolysis products
E_j	activation energy for reaction j
f_i	mol fraction of species i
F	incidence matrix of process constraints
F_m	constraint vector involving measured variables only
F_z	partial derivative of constraint vector with respect to the measured variables
F_θ	partial derivative of constraint vector with respect to the parameters to be estimated
F_i	mass flowrate of species i
g	mass fraction of species i in air fed to gasifier
G	Gibb's free energy
G_o	vector of discrepancies of measured data from satisfaction of constraints
G_1	vector of discrepancies after some data adjustment
ΔH_j	enthalpy change of reaction j
h_w	overall heat transfer coefficient across inner wall of gasifier
h_{wo}	overall heat transfer coefficient across outer wall of gasifier
k_e	effective axial heat transfer coefficient
k_g	thermal conductivity of gas mixture
k_s	thermal conductivity of the solid
k_p	mass transfer coefficient
k_{rj}	intrinsic reaction rate

k_w thermal conductivity of the gasifier wall

L height of the packed bed

m number of constraints
M_I molecular weight of species I

N normalized version of A test statistic
N_{Gr} Grashof Number
N_{Pr} Prandtl Number
N_{Re} Reynolds Number

p number of parameters θ to be estimated
P pressure
P_i partial pressure of species I

P_I^{eq} equilibrium partial pressure of species I

Q $= (F_z R F_z^T)^{-1}$

r radius of inner wall of gasifier
r_o radius of outer wall of gasifier
r^f fractional radius of partially reacted particle
R universal gas constant
R variance-covariance matrix of the measured data (Section 4.3)
R_d diagonal variance matrix of measured data
R_j^d apparent rate of reaction j
R_c^j pyrolysis distribution constant
R_c^h pyrolysis distribution constant

T local temperature
T_a temperature in the annulus at the same axial position as T
T_c temperature in the bed at the same axial position as T
T_{amb} ambient temperature

U $= dT/dz$

w half-width of the combustion zone
W mass of the particle at time t
W_o initial mass of the particle when wet
W_1^o mass of the particle when drying is complete but pyrolysis has not yet commenced

X_i mol fraction of species I in pyrolysis products
X_C, X_O, X_H overall elemental composition of pyrolysis products (mol fraction)
X, X_1 conversion of solid particle in pyrolysis and gasification

z axial position in the gasifier (measured from the top of the bed)
Z_o measured data vector
Z_1^o adjusted data vector
Z_{i+1} solution vector for adjusted data set = $\hat{Z}$

θ	parameter vector
λ	stoichiometric coefficient for combustion reaction 3d
μ	viscosity
ρ	density
σ	standard deviation
$\| \|$	Euclidean norm

Subscripts

g	gas
i	C, H_2O, H_2, CH_4, CO, CO_2, O_2, N_2
j	1, 2, 3a, 3b, 3c, 3d, 4, 5, 6
s	solid

Superscripts

o	initial/feed conditions
P	pyrolysis
^	adjusted data set

Throughout this report the units for all measures are in appropriate combinations of Joules, meters, kilograms, Kelvin, and seconds unless otherwise specified.

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Appendix A.1.1 : Calculation of the Elemental Composition of the Pyrolysis Products

Given the ultimate and proximate analyses for dry wood:

ULTIMATE ANALYSIS		PROXIMATE ANALYSIS	
f_c°	carbon	f_{fc}°	fixed carbon
f_h°	hydrogen	f_v°	volatiles
f_o°	oxygen	f_a°	ash

the elemental composition of the gaseous pyrolysis products is computed as:

$$f_c^P = f_c^\circ - f_{fc}^\circ$$

$$f_h^P = f_h^\circ$$

$$f_o^P = f_o^\circ$$

All values are on a mass fraction, dry wood basis. The atomic weight fraction equivalents of f_c^P, f_h^P and f_o^P are X_C^P, X_H^P and X_O^P, respectively.

Appendix A.1.2: The Rate Equation for the Shrinking Unreacted Core Model

In the shrinking unreacted core model, the diffusion of reactants through the external ash layer to the reaction interface is included as an extra resistance to reaction. The char particle is considered one-dimensional in this model because the grain structure of wood and wood char is largely one-dimensional. Reaction is considered to be limited to the cross-grain faces of the particle. Thus, the SCM, developed on the basis of a flat particle of halfwidth L in the grain direction is:

$$R_i = \frac{(1-\varepsilon)\ (P_I - P_i^{eq})}{\frac{L}{k_p} + \frac{L^2(1-r_f)RT}{D_e} + \frac{(P_i - P_i^{eq})}{r_f\ \eta\ k_r}}$$

where η = the reaction effectiveness factor

$$= \frac{1}{\phi}\ \tanh(\phi)$$

and ϕ = the Thiele modulus

$$= \left(\frac{k_r L^2}{D} \right)^{1/2}$$

Appendix A.2 : Physical Properties

The physical properties package is largely the same as that used in our previous project (ENFOR C-39) in which a mechanistic model was developed for fluidized bed wood gasifiers [45]. The details of this package are summarized below.

A.2.1 THERMAL CONDUCTIVITY

WOOD [46]

$$k = S_g(1.39 + 0.028\ M) + 0.165 \qquad \text{for } M < 40 \text{ wt\%}$$

$$= S_g(1.39 + 0.038\ M) + 0.165 \qquad \text{for } M > 40 \text{ wt\%}$$

where k is the thermal conductivity (BTU in/ft^{2}hr°F)
M is the moisture content of the wood (wt%)
S_g is the specific gravity of the wood based on oven dry volume

CHAR [47]

$$k = 0.02 + 1.25 \times 10^{-5}\ T \qquad (W\ cm^{-1}\ K^{-1})$$

GASES [48]

$$k = a + bT + cT^2 \qquad (W\ m^{-1}\ K^{-1})$$

(see Table 9 for coefficients a,b,c)

MIXING RULE for the thermal conductivity of a gas mixture [30]

$$k_{mix} = \frac{\Sigma\, x_I k_i (M_I^{1/3})}{\Sigma\, x_i (M_I^{1/3})}$$

where x_I is the mol fraction of I in the gas phase

M_I is the molecular weight of I

Table 9 : Thermal Conductivity Coefficients [48]

Gas	$ax10^2$	$bx10^3$	$cx10^7$	σ^2x10^7	Range (K)
H_2O	-3.15333	0.145714	-0.266667	8.0953	600- 900
H_2	7.777198	0.362363	-0.120879	6.3573	600-1250
CH_4	0.00994014	0.0772505	0.818226	0.33827	600-1250
CO	1.10418	0.059247	-0.057967	0.5606	600-1250
CO_2	-1.95682	0.119447	-0.317582	1.31069	600-1250
O_2	0.618402	0.0763505	-0.108331	0.58415	600-1090
N_2	0.939180	0.0642581	-0.105185	0.32876	600-1250

A.2.2 VISCOSITY

GASES [49]

$$\mu = a + bT$$

where μ is the viscosity of the gas (N s m^{-2})
T is the temperature (K)
(see Table 10 for the coefficients a and b)

except for steam, where

$$= [80.4 + 0.407(T - 273.15)] \times 10^{-7} \quad (N\ s\ m^{-2})$$

MIXING RULE for the viscosity of a gas mixture [30]

$$\mu_{mix} = \frac{\Sigma\, x_i \mu_i (M_i^{1/2})}{\Sigma\, x_i (M_i^{1/2})}$$

where x_i is the mol fraction of i in the gas phase
M_i is the molecular weight of i

Table 10 : Viscosity Coefficients [49]

Gas	a x 10^6	b x 10^6	$\sigma^2 \times 10^6$	Range (K)
H_2	5.579	0.0151	0.004	300-1300
CH_4	7.384	0.0204	0.017	300-1300
CO	14.380	0.026	0.097	300-1300
CO_2	10.389	0.029	0.118	300-1300
O_2	15.651	0.0327	0.194	300-1300
N_2	14.389	0.0257	0.092	300-1300

A.2.3 HEAT CAPACITY

WOOD [46]

$$C_p = 0.266 + 0.00116\ (T - 273.15)$$

where C_p is the heat capacity of wood (cal g^{-1} K^{-1})

for 273 K < T < 379 K

The heat capacity of wood is reported to be affected by moisture content and slightly by specific gravity but quantification of these effects has not been found in the literature.

CHAR AND GASES [14]

$$C_p = a + bT + cT^{-2} + dT^2 \qquad (\text{cal mol}^{-1}\ K^{-1})$$

where coefficients a,b,c,d are in Table 11.

Table 11 : Heat Capacity Coefficients [14]

Species	a	$bx10^{3}$	$cx10^{-5}$	$dx10^{6}$	Range(K)
Char(Carbon)	4.03	1.14	-2.04		298-2500
$H_2O(g)$	7.30	2.46			298-2750
H_2	6.52	0.78	0.12		298-3000
CH_4	3.381	18.044		-4.300	298-1000
CO	6.79	0.98	-0.11		298-2500
CO_2	10.57	2.10	-2.06		298-2500
O_2	7.16	1.00	-0.40		298-3000
N_2	6.83	0.90	-0.12		298-3000

A.2.4 DIFFUSIVITY

Binary diffusion coefficients are computed using the Wilke-Lee modification [50] of the equation by Hirshfelder, Bird and Spotz [51]. Accuracy of this correlation is reported as 7 to 8%.

$$D_{ab} = \frac{B\ T^{3/2}\ (1/M_a + 1/M_b)^{1/2}}{P\ r_{ab}^{2}\ I_D}$$

where D_{ab} is the binary gas diffusivity ($cm^2 s^{-1}$)

$B = [10.85 - 2.50(1/M_a + 1/M_b)^{1/2}] \times 10^{-4}$

T is the local temperature (K)

M_a, M_b are the molecular weights of a and b

P is the absolute pressure (atm)

r_{ab} is the collision diameter (Å) $= \frac{(r_{oa} + r_{ob})}{2}$

r_o (see Table 12)

I_D is the collision integral for diffusion (see Table 13)

$\varepsilon_{ab}/k = [(\varepsilon_a/k)(\varepsilon_b/k)]^{1/2}$

(see Table 12)

k is the Stephan Boltzmann constant

$= 1.38 \times 10^{-6}$ (erg K^{-1})

ε_{ab} is the energy of molecular interaction (ergs)

MIXING RULE for the steady state diffusion of one component through a multi-component mixture [30]

$$D_{a,mix} = \frac{1 - x_a}{(x_b/D_{ab} + x_c/D_{ac} + x_d/D_{ad} + \ldots)}$$

Table 12 : Force Constants and Collision Diameters [50]

Gas	ε/k (K)	r_o (Å)
H_2O	363	2.655
H_2	33.3	2.968
CH_4	136.5	3.882
CO	110.3	3.590
CO_2	190	3.996
O_2	113.2	3.433
N_2	91.5	3.681

Table 13 : The Collision Integral [51]

kT/ε_{ab}	I_D	kT/ε_{ab}	I_D	kT/ε_{ab}	I_D
0.3	1.331	2.2	0.5203	9	0.3778
0.4	1.159	2.4	0.5061	10	0.3712
0.5	1.033	2.6	0.4939	20	0.3320
0.6	0.9383	2.8	0.4836	30	0.3116
0.7	0.8644	3.0	0.4745	40	0.2980
0.8	0.8058	3.2	0.4664	50	0.2878
0.9	0.7585	3.4	0.4593	60	0.2798
1.0	0.7197	3.6	0.4529	70	0.2732
1.1	0.6873	3.8	0.4471	80	0.2676
1.2	0.6601	4.0	0.4418	90	0.2628
1.3	0.6367	4.2	0.4370	100	0.2585
1.4	0.6166	4.4	0.4326	200	0.2322
1.5	0.5991	4.6	0.4284	300	0.2180
1.6	0.5837	4.8	0.4246	400	0.2085
1.7	0.5701	5.0	0.4211		
1.8	0.5580	6	0.4062		
1.9	0.5471	7	0.3948		
2.0	0.5373	8	0.3856		

A.2.4.1 EFFECTIVE DIFFUSIVITY IN WOOD CHAR

Groeneveld [4] reports data for the effective diffusivity of gas in wood char. His results are correlated as shown below.

$$D_e = D \times (7.69\ \varepsilon_p - 5.62) \qquad 0.75 < \varepsilon_p < 0.84$$

$$D_e = D \times \varepsilon_p \qquad 0.84 < \varepsilon_p < 1.00$$

where D_e is the effective diffusivity ($cm^2 s^{-1}$)

ε_p is the void fraction of the wood char particle

Appendix A.3 : Input Data for the Simulation Program

The following data were used for input to the simulation program:

OPERATING CONDITIONS ----------

* wood feed rate (wet basis)(kg/s)		= 0.02
* moisture content of wood (dry wood basis)		= 15 %
* wood particle dimensions (m)	length	= 0.025
	height	= 0.038
	width	= 0.089
* air feed rate (wet basis)(kg/s)		= 0.02
* air feed temperature (K)		= 348
* air feed composition (mass fraction,wet basis)	O_2	= 0.233
	N_2	= 0.767
	H_2O	= 0.000

GASIFIER DESIGN PARAMETERS ----------

* air feed pressure (atm)	= 1
* gasifier bed height (m)	= 1.6
* location of air tuyeres (m) (measured from top of bed)	= 1.2

ADJUSTABLE PARAMETERS ----------

* 1/2-width of combustion zone (m) = 0.03

FEED DATA ----------

* density of the wood (kg/m^3) = 480

* density of the packed bed (kg/m^3) = 290
  (based on void fraction = 0.4)

* proximate analysis of wood (mass fraction, dry wood basis)
  fixed C = 0.1982
  volatile = 0.7990
  ash = 0.0028

* ultimate analysis of wood (mass fraction, dry wood basis)
  C = 0.4922
  H = 0.0606
  O = 0.4444
  N = 0.0000

* void fraction in wood particle = 0.2

* ambient temperature (K) = 298

PARAMETERS FOR DGEAR ----------

* METH (drying zone) = 1
  (pyrolysis zone) = 2
  (combustion zone) = 2

* MITER = 3

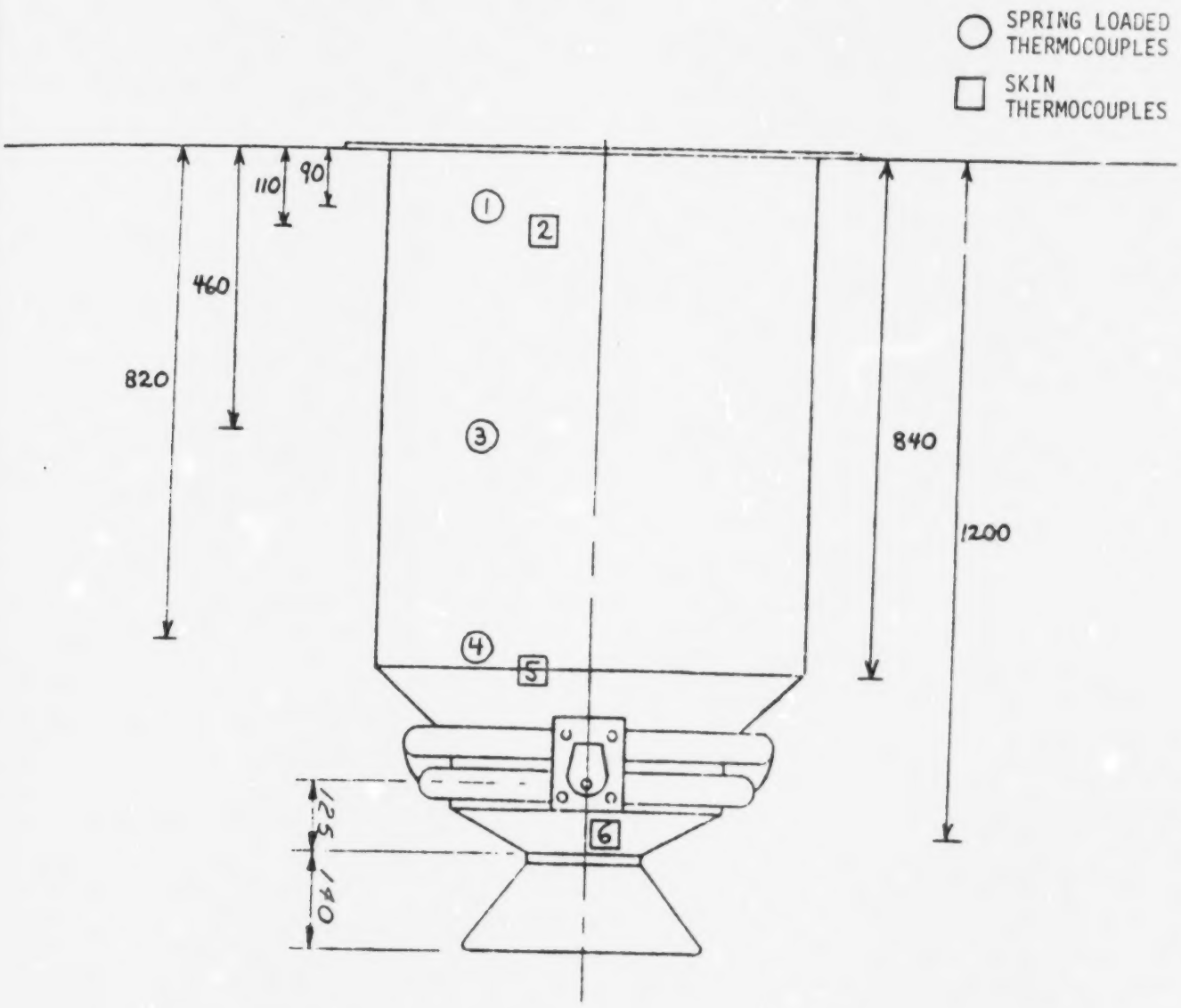
* H (drying zone) = 0.001
  (pyrolysis zone) = 0.00001

H	(combustion zone)	= 0.001
* TOL		= 1.0 E-6

Appendix A.4 : The SPC Data Set

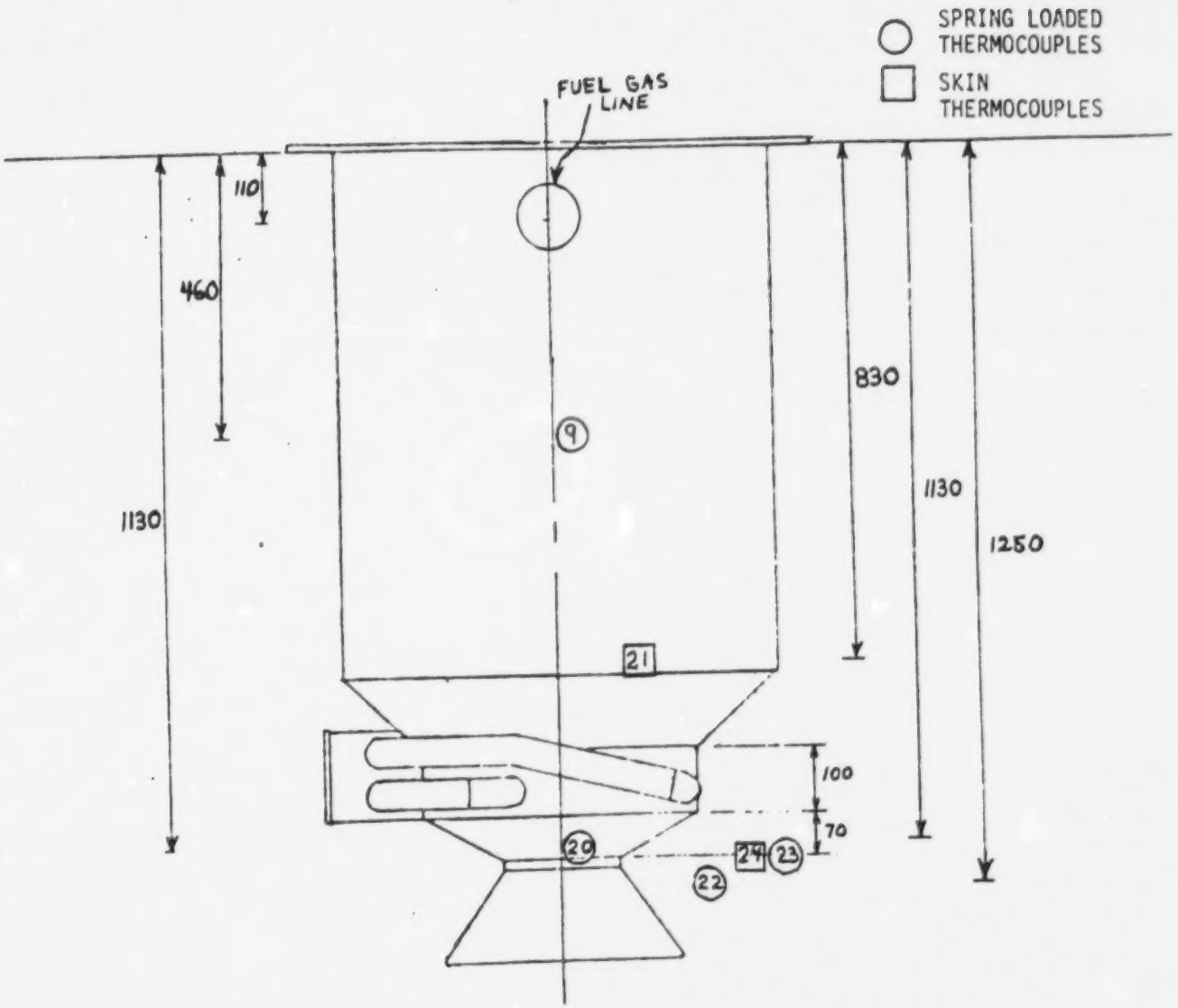
Table 14. SPC Datalogger Measurement Identification

Reference Number	Measurement
001	Temperature (°C)
002	Temperature (°C)
003	Temperature (°C)
004	Temperature (°C)
005	Temperature (°C)
006	Temperature (°C)
007	Temperature (°C)
008	Temperature at Hearth (°C)
009	Temperature (°C)
020	Temperature at Tuyere Level (°C)
021	Temperature (°C)
022	Temperature at Hearth (°C)
023	Temperature (°C)
024	Temperature (°C)
025	Temperature of Product Gas at Gasifier Exit (°C)
040	Temperature at Orifice for Gas Flow Measurement (°C)
041	Temperature of Preheated Air (°C)
042	Temperature in Proximity of Gasifier (°C)
046	Mol Fraction of CO from IR Analysis
047	Mol Fraction of CO2 from IR Analysis
048	Mol Fraction of CH4 from IR Analysis
049	Mol Fraction of H2O based on Saturation
060	Static Pressure Upstream of Orifice (kPa)
061	Differential Pressure Across Orifice (kPa)
062	Air Flow Rate to Gasifier (not calibrated) (L/min)
072	Gas Flow Rate from Orifice Meter (m^3/min)



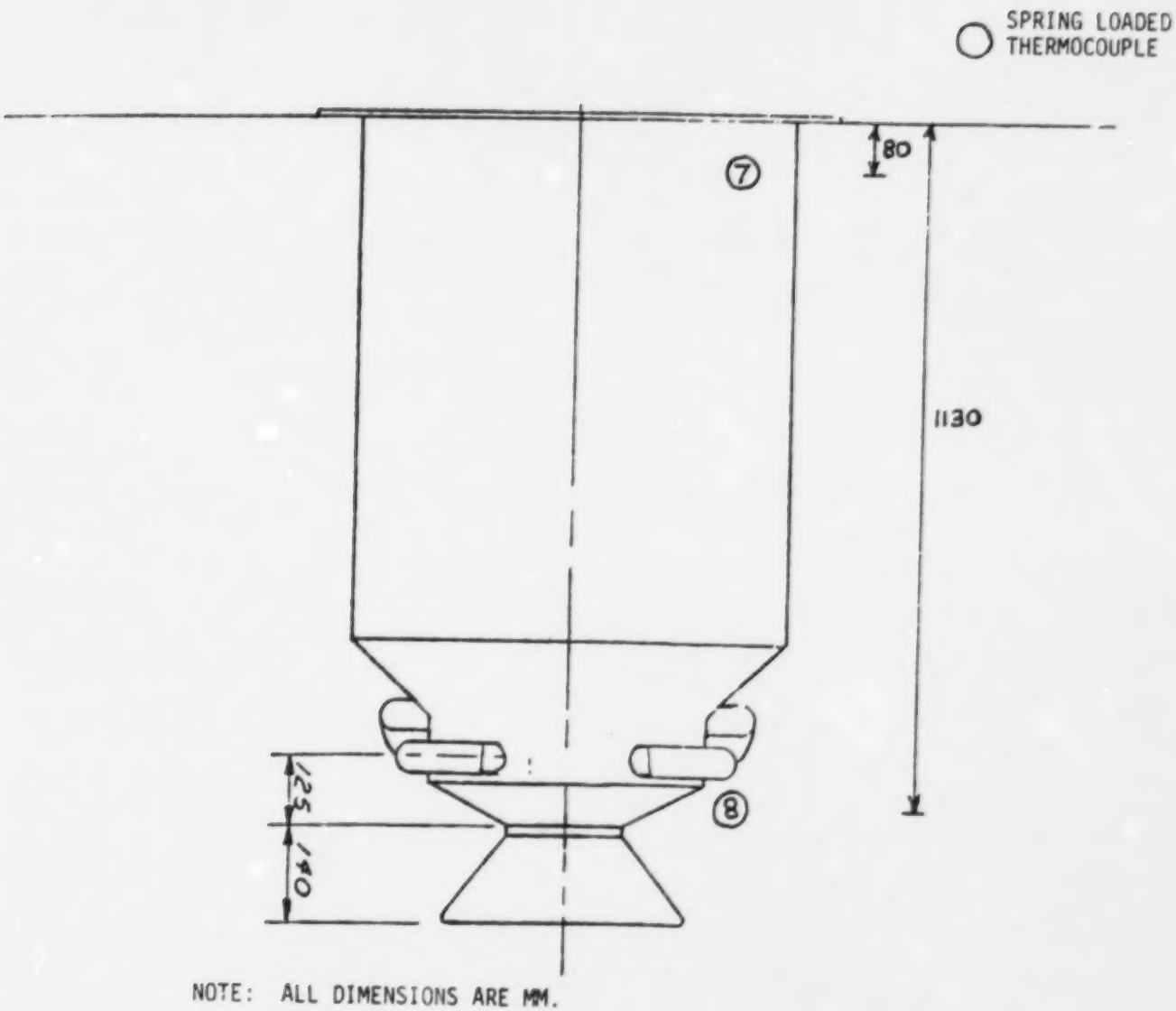
NOTE: ALL DIMENSIONS ARE MM.

Figure 17a : SPC Gasifier Thermocouple Locations (Front View) [33]



NOTE: ALL DIMENSIONS ARE MM.

Figure 17b : SPC Gasifier Thermocouple Locations (Side View) [33]



NOTE: ALL DIMENSIONS ARE MM.

Figure 17c : SPC Gasifier Thermocouple Locations (Rear View) [33]

Table 15. Steady State Values of the Measured Variables (SPC)

Run #	Wood Size	Wood Moist	Elect. Load	Air Temp	Grate Rotn	Measurement Reference Number* 062	072	040	060	H2	CO2	N2	CH4	CO
										------ GC ANALYSIS -------				
R8	52	15.4	33.6	102	4	980	2.32	314	97.7					
R10	52	14.5	33.6	124	4	971	2.17	309	97.5					
R11	38	10.9	33.6	147	5	1080	2.41	304	96.4					
R12	38	12.2	33.6	74	5	884	2.01	313	97.8	.177	.127	.496	.009	.19
R13	38	20.	34.0	12	5	1088	2.59	318	97.0	.189	.117	.473	.010	.20
R14	38	20.	25.6	75	3	858	1.95	313	97.8	.188	.131	.475	.013	.19
R15	38	13.7	34.4	70	3	970	2.35	316	100.4	.181	.108	.481	.012	.28
R16	52	15.	33.6	126	4	1056	2.44	316	97.0	.152	.140	.523	.012	.14
R17	52	15.	33.6	124	4	1108	2.29	321	97.1	.166	.138	.517	.007	.12
R19	52	15.	33.6	30	4	939	2.31	318	97.2	.183	.132	.502	.006	.17
R21	64	10.0	33.6	75	5	934	2.35	321		.191	.126	.475	.011	.19
R22	64	11.0	25.6	74	3	867	1.91	311	97.7	.195	.107	.472	.008	.28
R23	64	20.1	34.4	74	3	996	2.28	316	97.0	.192	.118	.480	.011	.19
R24	64	20.	25.6	74	5	1034	2.18	311	96.9	.196	.127	.463	.009	.16
R25	52	15.	48.8	131	4	1171	2.49	316	96.2	.195	.132	.470	.011	.19
R26	52	15.	18.4	28	4	833	1.64	294	98.3	.205	.122	.474	.010	.19
R28	52	25.	33.6	125	4	1043	2.29	319	96.9	.206	.141	.466	.012	.16
R29	52	15.	34.0	122	4	1105	2.53	319	96.6	.204	.113	.503	.000	.18
R30	52	15.	33.6	125	2	1085	2.30	319	97.0	.204	.112	.464	.013	.26
R31	52	15.	33.6	123	6	982	2.15	320	97.1	.189	.121	.485	.009	.19
R32	52	15.	33.6	126	4	986	2.18	321	97.2	.163	.131	.488	.014	.20
R34	25	15.	33.6	126	4	1013	2.45	316	96.6	.163	.130	.508	.010	.18
R35	89	15.	33.6	123	4	1094	2.65	319	96.4	.137	.135	.595	.000	.12
R37	38	20.	34.2	173	3	940	2.64	320	96.1	.172	.140	.504	.011	.14
R38	64	20.	26.4	175	3	857	2.37	318	96.7	.160	.141	.514	.010	.16
R39	64	20.	36.0	109	5	970	2.74	315	94.9	.163	.141	.511	.011	.15
R40	64	12.3	33.6	173	3	1160	2.73	314	94.0	.154	.132	.519	.008	.18
R41	64	12.1	25.6	172	5	927	2.26	316	95.9	.158	.140	.515	.011	.16
R42	38	12.7	25.6	173	3	783	1.92	311	95.4	.160	.138	.510	.011	.18
R43	38	20.	25.4	173	5	925	2.31	311	94.2	.186	.133	.483	.011	.18
R44	52	14.6	34.4	198	4	867	2.26	316	94.9	.176	.127	.498	.011	.18

* refer to Table 14 for an explanation of the Measurement Reference Numbers

Table 15. Steady State Values of the Measured Variables (SPC) (cont'd)

Run #	Measurement Reference Number														
	001	002	003	004	005	006	007	008	009	020	021	022	023	024	025
R8	204	148	311	498	275	425	151	809	395	591	237	919	306	176	422
R10	155	86	242	430	186	348	153	826	418	544	236	924	325	205	411
R11	171	140	262	435	235	370	123	845	141	658	246	945	347	169	461
R12	153	99	254	456	224	329	135	830	75	556	229	933	310	213	427
R13	178	106	248	313	464	217	364	124	881	610	228	956	313	187	451
R14	144	98	268	413	212	353	130	797	52	506	184	866	300	154	391
R15	177	106	266	466	214	357	135	832	98	584	215	927	299	198	428
R16	183	104	300	478	194	367	153	841	169	681	233	878	320	229	457
R17	157	110	286	456	223	387	190	824	115	658	239	914	324	219	473
R19	133	108	262	441	249	369	147	810	197	665	237	916	301	169	457
R21	220	171	312	499	261	394	140	866	140	598	211	920	360	187	449
R22	156	81	223	412	161	270	119	821	198	671	201	917	343	105	449
R23	192	114	249	456	201	369	137	846	113	678	213	936	367	217	470
R24	188	131	276	459	203	25	129	847	116	694	184	920	358	197	457
R25	202	153	286	478	246	34	132	854	76	681	208	912	359	196	481
R26	160	102	233	410	193	41	127	816	86	576	182	900	294	157	416
R28	202	156	275	453	230	39	164	809	102	604	189	935	312	190	440
R29	195	117	290	461	191	36	83	459	168	653	204	985	343	182	478
R30	198	160	282	444	231	46	145	866	172	662	201	982	297	154	483
R31	196	143	318	498	243	58	149	947	165	713	202	1007	288	158	503
R32	182	132	272	487	220	37	170	980	214	765	215	1057	124	163	511
R34	122	119	177	361	178	320	156	773	70	618	250	816	328	202	472
R35	117	72	182	395	176	52	167	786	144	697	289	841	351	235	508
R37	134	81	202	391	166	38	155	823	143	633	267	838	353	217	460
R38	217	192	346	557	294	83	170	814	250	671	235	827	348	216	485
R39	206	188	417	605	368	44	164	843	109	702	254	838	335	181	516
R40	195	140	375	607	324	30	165	877	95	769	263	894	371	209	524
R41	142	114	244	450	242	43	149	842	127	761	216	761	333	173	502
R42	114	94	155	316	174	34	132	802	143	743	241	790	295	157	493
R43	216	172	342	535	289	39	142	884	131	775	233	844	322	117	492
R44	118	78	182	368	186	37	142	869	143	782	249	879	234	168	507
Avg	172	123	269	458	226	361	147	841	152	663	226	901	329	184	467

Table 16. Standard Deviations of the Measured Variables (SPC)

Run #	Measurement Reference Number 062	072	040	060
R8	55	0.82	1	0.20
R10	74	0.18	1	0.35
R11	150	0.26	32.4	8.11
R12	30	0.37	1	0.20
R13	131	0.30	1.9	1.03
R14	153	0.08	1.0	0.19
R15	160	0.13	22.5	26.0
R16	68	0.16	1.0	0.33
R17	73	0.11	1	0.37
R19	70	0.14	1	0.28
R21	39	0.0	0	0.71
R22	39	0.07	1	0.10
R23	135	0.27	1	0.20
R24	44	0.08	1	0.31
R25	126	0.14	0.4	0.41
R26	382	0.64	2.7	0.98
R28	52	0.13	0.7	0.32
R29	58	0.11	1	0.33
R30	58	0.15	0.9	0.29
R31	139	0.15	1	0.39
R32	52	0.10	1	0.22
R34	53	0.13	1	0.31
R35	112	0.20	0	0.50
R37	87	0.15	0.6	0.42
R38	184	0.34	1	0.68
R39	225	0.69	1	1.38
R40	72	0.18	1	0.86
R41	87	0.22	1.2	0.56
R42	126	0.25	1	0.33
R43	152	0.29	0.4	0.58
R44	93	0.13	1.0	0.44

Table 16. Standard Deviations of the Measured Variables (SPC) (cont'd)

Run #	Measurement Reference Number														
	001	002	003	004	005	006	007	008	009	020	021	022	023	024	025
R8	8.9	11.0	5.4	18.4	9.7	13.2	7.8	21.0	4.9	17.7	5.0	17.1	7.3	5.6	9.2
R10	7.4	6.8	2.5	6.8	11.0	9.8	3.6	17.9	4.8	9.6	4.6	8.5	8.5	4.4	12.4
R11	14.5	9.2	4.9	22.6	6.1	30.8	6.4	34.4	21.5	17.4	4.8	17.2	7.9	4.5	9.2
R12	10.3	7.7	10.4	19.3	8.3	11.1	6.3	21.9	4.9	16.4	5.8	24.7	7.4	21.8	10.3
R13	15.7	16.4	9.1	11.9	30.1	21.3	21.9	8.0	27.1	19.7	7.7	24.4	11.9	14.4	17.1
R14	20.1	15.0	19.9	24.2	16.1	8.2	16.8	25.1	4.6	23.9	39.4	24.1	10.8	7.6	18.2
R15	17.5	12.2	18.4	18.9	11.9	18.8	23.7	33.7	8.7	28.6	8.7	27.0	12.3	6.9	23.7
R16	6.4	6.3	19.7	41.2	16.1	16.5	13.9	27.2	51.1	23.8	8.4	190	8.0	15.9	16.3
R17	9.9	6.2	9.5	22.0	18.1	13.3	19.6	21.6	10.7	15.3	2.8	12.0	5.3	7.8	14.3
R19	7.6	6.0	8.1	14.8	4.9	8.9	20.0	21.8	29.9	28.3	3.1	21.9	9.4	1.9	26.8
R21	5.6	6.4	5.1	12.3	40.5	8.7	2.9	29.9	15.2	9.3	2.4	11.1	3.4	12.9	
R22	17.9	6.5	3.9	17.5	8.9	9.6	11.7	21.3	15.3	20.0	3.7	13.9	14.2	8.8	14.5
R23	9.8	3.4	8.2	10.8	12.0	19.7	11.6	32.9	13.0	22.7	11.2	12.8	13.8	12.0	24.5
R24	10.0	4.5	9.9	16.7	13.5	3.6	12.9	23.1	16.9	28.4	6.3	20.4	11.4	9.4	21.5
R25	17.4	12.3	13.8	15.8	9.8	4.3	17.6	33.5	6.5	31.0	6.6	186	14.4	9.4	31.0
R26	12.8	10.2	15.2	16.0	9.8	9.3	10.9	13.7	8.5	9.5	4.4	18.7	24.1	6.1	4.6
R28	9.5	12.2	7.9	13.3	5.7	4.7	10.3	27.8	32.9	11.3	7.6	23.8	15.8	6.5	14.1
R29	7.2	10.6	7.1	11.3	15.4	2.8	21.3	11.2	12.2	13.5	5.4	25.1	13.1	5.4	9.8
R30	8.1	5.8	12.8	20.5	9.3	5.5	7.9	28.1	21.4	11.9	3.2	17.6	6.7	4.1	8.9
R31	11.4	9.4	8.0	16.8	10.2	2.8	17.2	52.6	18.6	26.5	58.6	210	59.4	19.4	11.0
R32	6.5	11.6	12.8	19.4	11.4	2.6	9.4	53.9	19.3	27.8	4.2	22.4	88.9	14.4	5.5
R34	6.9	6.3	5.7	15.1	8.0	16.6	3.9	23.6	8.1	15.0	2.8	7.8	5.3	20.6	8.7
R35	6.7	8.4	16.0	21.3	19.8	5.5	14.4	24.9	23.7	23.4	11.6	10.2	11.3	29.6	9.1
R37	12.3	14.6	28.7	39.2	8.9	1.8	17.0	22.1	19.6	31.0	9.0	14.2	6.9	10.5	14.3
R38	12.0	8.9	18.7	31.4	14.2	6.0	9.4	18.7	56.1	30.2	62.7	25.0	9.1	12.1	17.4
R39	17.2	8.6	34.7	35.2	11.5	5.2	8.4	28.8	9.7	41.2	12.1	30.2	45.2	13.8	14.9
R40	8.6	15.5	33.6	41.7	26.3	11.8	11.8	31.0	11.2	30.5	10.0	11.8	5.0	18.9	24.9
R41	12.3	14.6	28.7	39.2	8.9	1.8	27.6	19.9	91.7	23.7	8.1	18.8	10.4	10.5	20.9
R42	6.4	5.8	10.1	19.6	8.7	3.5	8.1	28.7	13.5	32.4	8.9	18.5	53.2	8.2	14.2
R43	10.9	7.2	13.5	17.5	26.9	1.8	17.0	22.1	19.6	31.0	9.0	14.2	22.3	3.7	14.2
R44	6.6	9.5	12.6	18.1	12.7	5.2	8.7	21.8	15.6	33.6	19.7	20.0	142	4.8	18.6

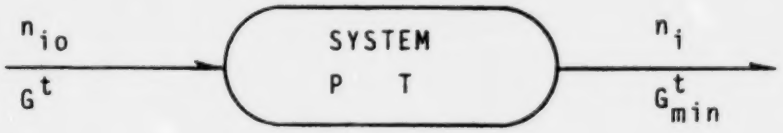
Table 17. Down Draft Gasifier Performance Measures: Experimental (Measured) Values (SPC)

Run #	GAS RATE	GAS TEMP	MAX TEMP	HHV	CO/H2
12	2.01	427	933	4.62	1.09
13	2.59	451	956	5.00	1.11
16	2.44	457	878	4.23	1.15
17	2.49	473	914	4.19	1.04
22	1.91	449	917	5.09	1.12
23	2.28	470	936	4.95	1.04
24	2.18	457	920	4.89	1.00
25	2.49	481	912	4.90	0.99
29	2.53	478	985	4.47	0.88
30	2.30	483	982	5.24	1.01
37	2.64	460	838	4.43	1.01
38	2.37	485	827	4.27	1.10
40	2.73	524	894	4.27	1.22
41	2.26	502	761	4.28	1.11
43	2.31	492	844	4.69	0.98

Appendix A.5 : Chemical Equilibrium

Only the water-gas shift reaction is assumed to be at equilibrium. However, the potential equilibrium state that could be achieved at the local conditions of temperature, pressure and composition in the bed is computed to determine the driving force for each chemical reaction considered in the mechanistic model.

Chemical equilibrium has been computed, as it was in our previous modelling project [45], by minimizing the total Gibbs free energy of the system. Consider the following system:



where n_{io} = inlet molar flow of species i into the system
n_i = molar flow of species i, corresponding to the equilibrium mixture, leaving the system
G^t = total free energy as a function of n_{io}, n_i and T

The system in this case is a compartment in the packed bed of the down-draft gasifier. With a given set of values P, T, and n_{io}, the equilibrium composition is obtained by minimizing G^t with respect to n_i, subject to the element balance constraints.

Let A_k = total number of atomic weights of the k^{th} element present in the system, as determined by the initial constituents of the system;

a_{ik} = number of atoms of the k^{th} element present in each molecule of chemical species i;

λ_k = undetermined Lagrange multipliers.

Then the element balance gives

$$\sum_i n_i \, a_{ik} = A_k \qquad k = 1, \ldots, W$$

Incorporating the above constraints in the minimization scheme, we can write the objective function F as

$$F(n_i, \lambda_k; P, T, n_{io}) = G^t + \sum_k \lambda_k \left(\sum_i n_i \, a_{ik} - A_k\right) \qquad (1)$$

The solution of equation (1) has been given by Smith and Van Ness [14]

$$\Delta G^\circ_{fi} + RT \ln (y_i \phi_i P) + \sum_k \lambda_k \, a_{ik} = 0 \qquad i = 1, \ldots N \qquad (2)$$

where ΔG°_f is the free energy of formation at T, which can be evaluated from the equation,

$$\Delta G^\circ_{fi} = (\Delta G^\circ_{fi})_{298K} - RT \int_{298K}^{T} \frac{(\Delta H^\circ_i)_{298K} + \int_{298}^{T} \Delta C_{pi} \, dT}{RT^2} \, dT \qquad (3)$$

where

$(\Delta H^\circ_i)_{298K}$ = heat of formation of species i at 298K

ΔC_{pi} = $C_{pi} - \sum_k C_{pk}$ (sum of pure elements contained in the species i)

P = total pressure in atmospheres

$\hat{\phi}_i$ = partial fugacity coefficient of component i in the

gaseous mixture

y_i = mol fraction of species i in the gas.

The solution of equation (2) gives the desired equilibrium composition. Equation (2), however, can be further simplified by assuming that the gases and their mixture are ideal.

$$\Delta G^{\circ}_{fi} + RT \ln (y_i P) + \sum_k \lambda_k a_{ik} = 0 \qquad (4)$$

Equation (4) represents a set of N+W simultaneous equations. The solution is complicated by the nonlinear logarithmic term, RT in $(y_i P)$, particularly when y_i has a very small value, which is often the case. The approach adopted for solving these equations is first to linearize in $(y_i P)$ by a first order Taylor series expansion followed by successive iterations of solving the linearized equations.

The solution of the linearized equations is obtained using the IMSL routine LEQT1F which was renamed LINEAR. This routine has the advantage of using minimal computer storage. The decomposition of the matrix is done by the Crout algorithm with optional accuracy test. The accuracy test determines whether the computed decomposition is accurate to a preassigned number of decimal places. We found that this test is not needed for our calculation, and it is by-passed by assigning a proper identification number.

The routine also tests the singularity of the matrix. When singularity exists, the computation is stopped and a message is printed. This occurs when any species in the system reduces to nearly zero. The problem is partially alleviated by setting a lower concentration limit. During the calculation, if the concentration of any gas species drops below this limit the concentration is automatically set at the lower limit.

Appendix A.6 : The Simulation Program

QUGAS2 Version 83-09

Appendix A.6.1: Simulation Program Description

In the down-draft gasifier simulation program QUGAS2, computation proceeds as follows:

1a. INITIAL ANNULAR PROFILE

* An annular profile is estimated for each of the independent variables. These annular conditions are used in computing heat transfer between the bed and the annulus. These initial annular profiles are used only in the first profile iteration, after which they are repeatedly updated with the most recent predictions from the model.

1b. GENERAL INITIALIZATION

* Initial values are estimated for each of the independent variables: mass flowrates of wood, water vapour, hydrogen, methane, carbon monoxide, carbon dioxide, oxygen and nitrogen, the temperature at the top of the bed and the temperature gradient at the top of the bed. The information which is used for the estimation of these initial values is outlined in Section 2.7.1.

* The dependent position variable z is initialized as zero at the top of the bed. z is equal to ZL at the grate level in the gasifier, where ZL is the vertical distance between the top of the bed and the grate. Grate level is considered to be the bottom of the gasifier in this model. After computation has reached the bottom of the gasifier (having completed evaluation within the moving bed), the numerical analysis turns around and continues by moving up in the annulus toward the top of the gasifier. z is

incremented to a final value of 2(ZL) at the top of the gasifier in the annulus. See Figure 18.

* A flag (ICOUNT) is set to indicate that computation is to start within the drying zone. ICOUNT is reset at intermediate stages within the simulation to indicate the reaction zone which governs behaviour at the local position within the gasifier.

ICOUNT=1	Drying (Reaction 1)
ICOUNT=2	Pyrolysis (Reaction 2)
ICOUNT=3	Pyrolysis is complete but combustion has not commenced yet (no reaction)
ICOUNT=4	Pyrolysis and combustion are proceeding simultaneously (Reactions 2,3a,3b,3c,3d,4,5,6,7)
ICOUNT=5	Combustion (Reactions 3a,3b,3c,3d,4,5,6,7)
ICOUNT=6	Gasification (Reactions 4,5,6,7)
ICOUNT=7	No further reaction (post-reaction zone)

* The parameters which are necessary for using DGEAR to solve the differential equations (METH,MITER,H,INDEX, TOL) are set. These are updated periodically as required. For example, at the top of the bed conditions change very slowly and the Adam's method of solution is sufficient. Lower in the bed, particularly in the combustion zone, conditions change very rapidly and the system of equations becomes stiff. In this region the Gear method [52] is necessary.

* When computation is proceeding within the bed, interpolation of the most recent annular profiles is performed (when ICOUNT=1,2,3,4,5 or 6). When computation is proceeding within the annulus (ICOUNT=7), interpolation of the most recent profiles

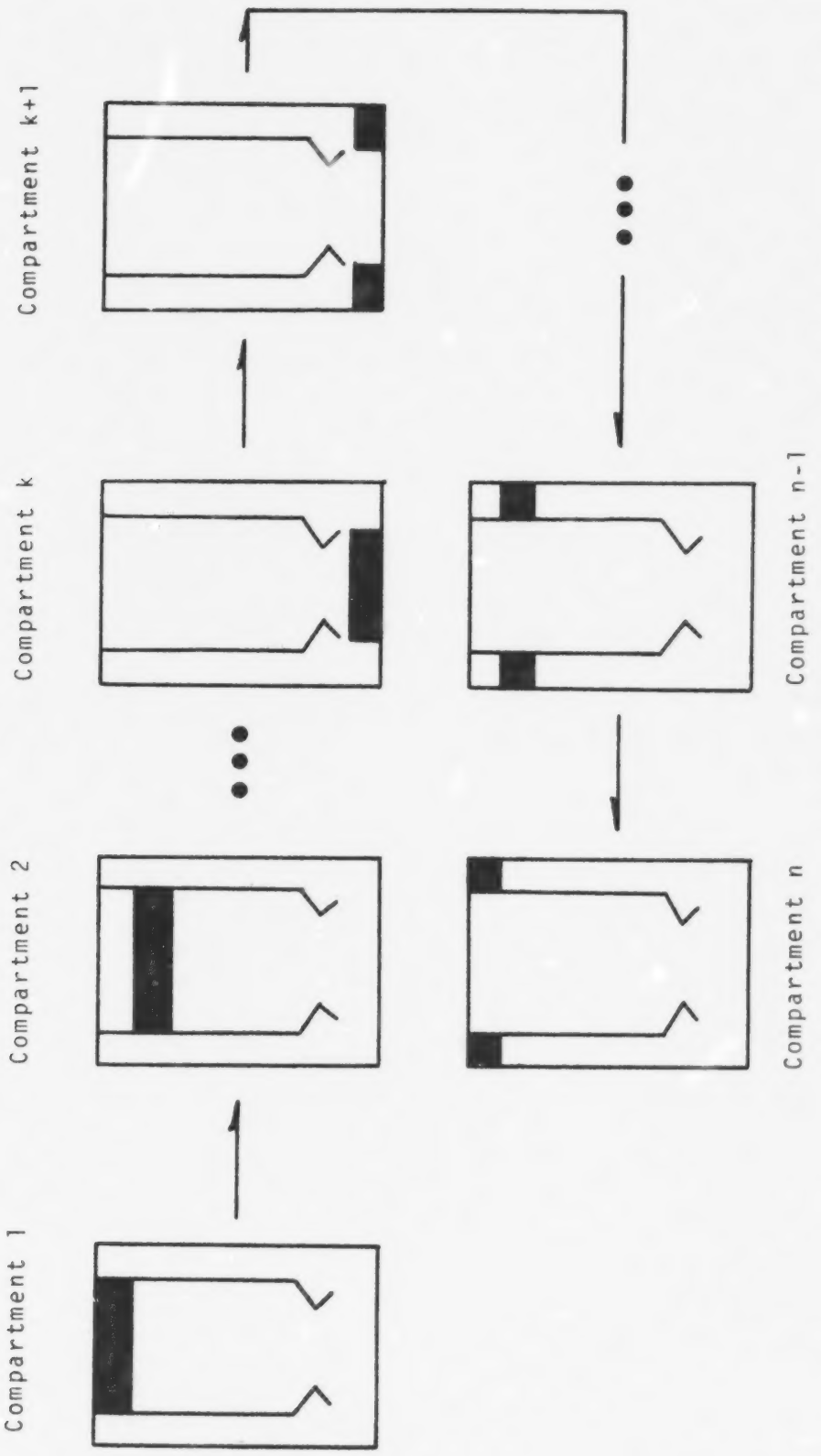


Figure 18: Progress of the Compartment Calculation

within the bed is performed. The purpose of this step is to produce a set of values that represent the conditions on the opposite side of the inner wall of the gasifier. Designation of "the opposite side" depends on which side of the wall computation is currently proceeding. These values are used to estimate the overall heat transfer coefficient across the wall.

2. ZONE COMPUTATIONS

* Compute the physical properties of the solid and gas at z. (subroutine PRPTYS)

* Compute the physical dimensions of the gasifier at z. (subroutine GEOMTY)

* Compute the heat transfer coefficients at z. (subroutine HTCOF)

* Set the size of the next compartment, Δz. An updated solution of the mass and energy balances will be computed at $z+\Delta z$ during the next call to DGEAR.

* Check the boundary condition for the current reaction zone.
    * If the reaction zone is not complete then continue, or
    * if the reaction zone is complete then reset the flag ICOUNT for the next reaction zone and continue.

* Compute the enthalpy change of reaction. (subroutine DELTAH)

* Set $z_{end}=z+\Delta z$ for use in DGEAR. DGEAR updates both the dependent and independent variables internally. Therefore, when control is returned to the MAIN

program the current value of z is equal to the value of $z+\Delta z$ before DGEAR was called.

3. CALL DGEAR
   * Within the control of DGEAR, subroutines RATE and FCN are called repeatedly until a converged solution is achieved at z_{end}.
      * Subroutine RATE computes the appropriate reaction rate.
      * Subroutine FCN contains the differential equations for the mass and energy balances, YPRIME(I) being the differential equation representing the mass balance for species I.

4. LISTING
   * Print the following values which represent the conditions at z_{end}:
      * reaction zone
      * compartment reference number
      * axial position in the gasifier
      * the temperature across the wall from position z
      * updated values of the independent variables at z_{end}

5. WATER-GAS SHIFT ADJUSTMENT
   * Check whether the reaction zone is either combustion or gasification.
      * If it is not, then continue, or
      * If it is, then compute an adjustment to the independent variables which accounts for the water-gas shift equilibrium. In version 83-09 of QUGAS2 this adjustment is computed outside of the differential equations and DGEAR.

6. UPDATE
   * Update the profile vectors (PROF1 to PROF10) with the

values of z_{end} and the independent variables at z_{end}.

7. PROFILE CHECK

* Check whether the current profile is complete.
    * If it is not then GO TO 2.
    * If it is complete then check for convergence by comparing selected values of temperature from this profile with similar values from the previous profile.
        * If the profile has not converged then GO TO 1b. No sophisticated convergence acceleration techniques are used in version 83-09.
        * If the profile has converged then continue.

8. OUTPUT

* Print the predicted intermediate and final results (subroutine OUTPUT) and STOP.

Appendix A.6.2 : Simulation Program Nomenclature

ALM01	log mean heat transfer area for inner wall
ALM23	log mean heat transfer area for outer wall
ALPHA	adjustable parameter for effective diffusivity in char
AMOLA	mol fraction of ash in wood (dry basis) (AMOLC,AMOLH,AMOLN,AMOLO are for carbon,hydrogen, nitrogen and oxygen, respectively)
AREAI	heat transfer area for inner surface of inner wall
AREAO	mass flow cross-sectional area
CCP	heat capacity of individual species
COMPN	moles of species
CONV1	conversion of wood in pyrolysis (mass basis)
CONV2	conversion of char in gasification (mass basis)
COSH	hyperbolic cosine
CPAIR	heat capacity of air
CPANN	heat capacity of individual species in annulus
CPAVAN	average heat capacity for gas mixture in annulus
CPAVCO	average heat capacity for solid/gas mixture in bed
CPCOR	heat capacity of individual species in bed
D	binary diffusivity
DIF	diffusivity of species in gas mixture
DEFF	effective diffusivity of species in wood char
DELH	enthalpy of reaction
DELTAZ	height of a compartment
DENSGA	density of gas in the annulus
DENSGC	density of gas in the bed
DENSB	density of the packed bed
DENSBO	density of the packed bed initially
DENSP	density of the solid
DENSPO	density of the solid (wood) initially
DEQ	equivalent diameter for heat transfer
DH	height of wood particle
DL	one-half width of wood particle,measured in grain direction
DP	spherical equivalent particle diameter
DW	width of wood particle
EMAS	mass fraction distribution of pyrolysis products
EMISS	emissivity
EMOL	mol fraction distribution of pyrolysis products
ETA	effectiveness factor for reaction in the char particle
FACTOR	constants used in calculation of water saturation
FAIR	mass flowrate of air injected to a compartment
FAIRIN	total air feed rate (mass basis)
FGOXY	oxygen in gaseous products (mass basis)
FLOWNT	total molar flowrate of gas
FSO	initial wood feed rate (wet basis)
FSTAR	initial solid mass flowrate - benchmark used in

computing conversion

GASFLO	total gas flowrate in annulus (molar basis)
GIBB	Gibb free energy for species
GR	Grashof number for outer wall to ambient
GRANNI	Grashof number for outer wall to annulus
GRANNO	Grashof number for inner wall to annulus
H	initial step size for numerical solution
HCOMBP	enthalpy of combustion of pyrolysis products @ 298K
HCOMBW	enthalpy of combustion of wood @ 298K
HCPDT1	
HCPDT2	enthalpy of heating wood and pyrolysis products
HCPDT3	to reaction temperature
HFCI	forced convection heat transfer coefficient for inner wall to annulus
HFCO	forced convection heat transfer coefficient for outer wall to annulus
HNC	natural convection heat transfer coefficient for outer wall to ambient
HPB	packed bed heat transfer coefficient for packed bed to inner wall
HRS	heat transfer coefficient for radiation between solid surfaces
HRV	heat transfer coefficient for radiation between voids
HW	overall heat transfer coefficient between packed bed and annulus
HWO	overall heat transfer coefficient between annulus and ambient
H2OSAT	water saturation pressure
ICOUNT	counter indicating local reaction zone
IER	flag for error messages
INDEX	status parameter for numerical solution
ITERAT	maximum number of complete profile iterations
IWK	work storage vector
IZ	maximum number of compartments per profile iteration
JJ	counter for number of pofile iterations
JL	counter for number of compartments
KAIR	thermal conductivity of air
KEFF	effective thermal conductivity in packed bed
KEO	static contribution to effective thermal conductivity
KGANN	thermal conductivity of gas mixture in annulus
KGCOR	thermal conductivity of solid/gas mixture in bed
KK	thermal conductivity of individual species
KP	mass transfer coefficient
KR	intrinsic rate coefficient
KS	thermal conductivity of solid
KW	thermal conductivity of wall of gasifier
K7	equilibrium constant for water-gas shift reaction

LAMBDA	stoichiometric coefficient for carbon in reaction
METH	solution method parameter
MIDDLE	parameter in the air distribution function
MITER	iteration method parameter
MOLWT	molecular weight of individual species
MWAIR	molecular weight of air
MWAVA	average molecular weight of gas in annulus
MWAVC	average molecular weight of gas in bed
N	number of differential equations to be solved
NC	moles of carbon (NH2O,NH2,NCH4,NCO,NCO2,NO2,NN2 refer to moles of water,hydrogen,methane,carbon monoxide, carbon dioxide,oxygen and nitrogen, respectively)
NPTSG	number of data points available for geometry interpolation
NPTSP	number of data points available for pyrolysis interpolation
OPPOSE	chemical composition on opposite side of inner wall
PHI	Thiele modulus
PMOL	gross elemental composition of pyrolysis products
PP	partial pressure of gaseous species
PPEQ	equilibrium partial pressure of gaseous species
PRAIR	Prandtl number for ambient conditions
PRANN	Prandtl number for annular conditions
PRCOR	Prandtl number for packed bed conditions
PRESS	pressure in gasifier
PROF1	profile storage for local mass flowrate of carbon (PROF2 to PROF9 are storage for water to wood, PROF10 is local temperature storage, PROF11 is local position storage)
PROXA	proximate analysis of wood (dry, mass basis) PROXC, PROXW, PROXV are for fixed carbon, moisture, and volatiles, respectively
R	global reaction rate
RAD0	radius of gasifier, inner surface of inner wall (RAD1,RAD2 and RAD3 refer to outer surface of inner wall,inner surface of outer wall and outer surface of outer wall, respectively)
REANN	Reynolds number in annulus
RECORE	Reynolds number in packed bed
RF	fractional radius of particle
RH	pyrolysis product distribution constant
RO	pyrolysis product distribution constant
SINH	hyperbolic sine
T	temperature
TAIR	air feed temperature
TAMB	ambient temperature
TANN	local temperature in annulus
TCHECK	temperature check for convergence of water-gas shift

	equilibrium adjustment
TCOR	local temperature in packed bed
TCORS	local temperature of solid in packed bed
TGUESS	initial guess for temperature at the top of the bed
TMAX	maximum temperature in the gasifier
TMAXO	maximum temperature from previous profile iteration
TOL	tolerance parameter for numerical solution
VELANN	gas velocity in annulus
VISAIR	viscosity of air
VISANN	viscosity of gaseous mixture in annulus
VISCOR	viscosity of gaseous mixture in packed bed
VOID	void fraction in packed bed
VOIDP	void fraction of solid particle
VVISC	viscosity of individual gaseous species
WIDTH	width of the air jet
WK	work storage vector
XG	mol fraction of species in gas
XI	mol ratio of carbon monoxide to carbon dioxide
XMOL	mol fraction of species
Y	independent variable (mass flowrates and temperature) (see Table)
YPRIME	differential of Y
YY	intermediate value of Y
Z	position of top of compartment for which numerical solution is desired (measured from top of bed)
ZAIR	position of tuyeres
ZEND	position of end of compartment for which numerical solution is desired
ZETA	magnitude of shift necessary for water-gas shift equilibrium (moles of CO)
ZL	total height of packed bed
ZUPPER	upper limit of air penetration in packed bed

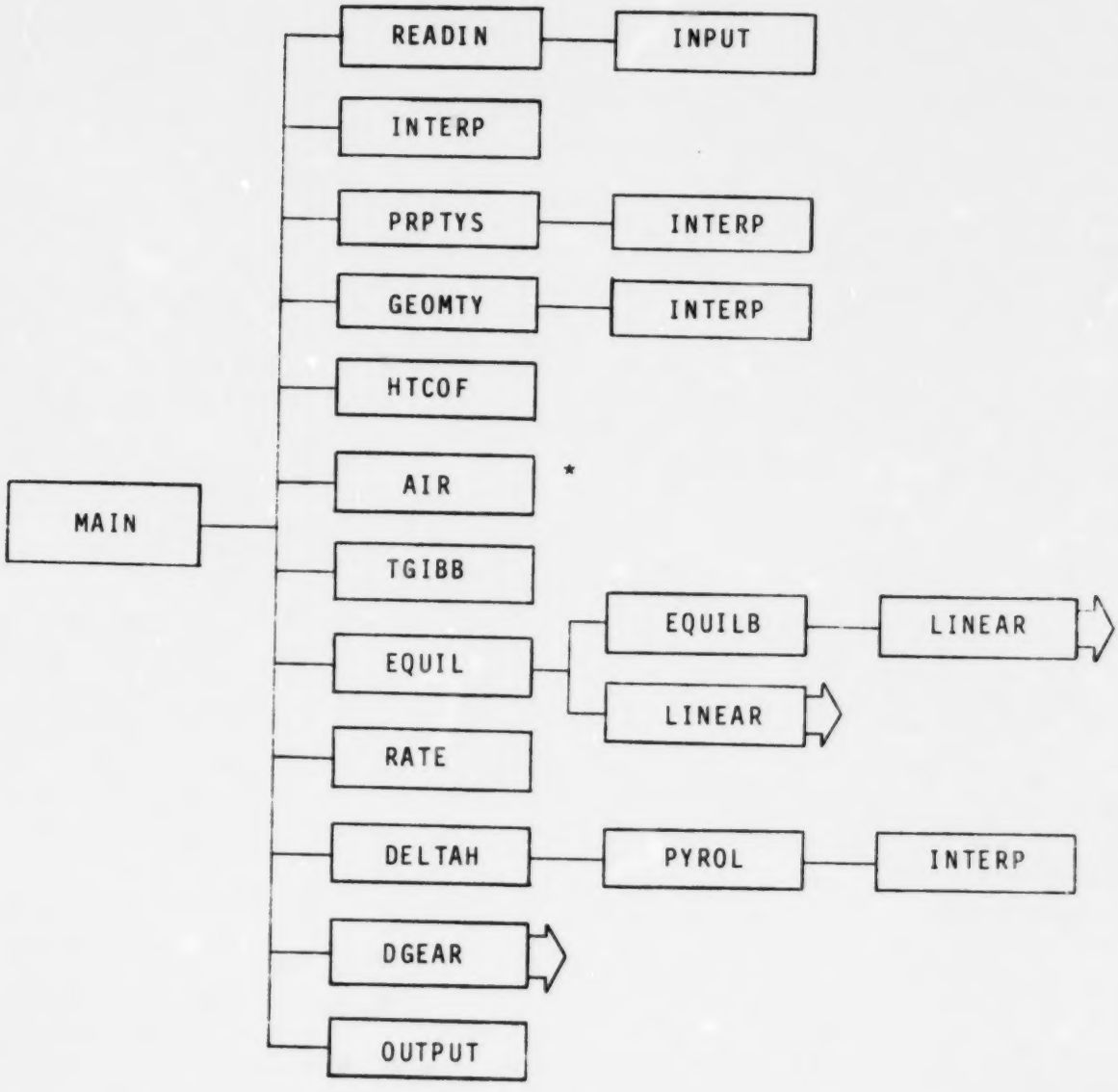


Figure 19 : Simulation Program Organization

* not in version 83-09.

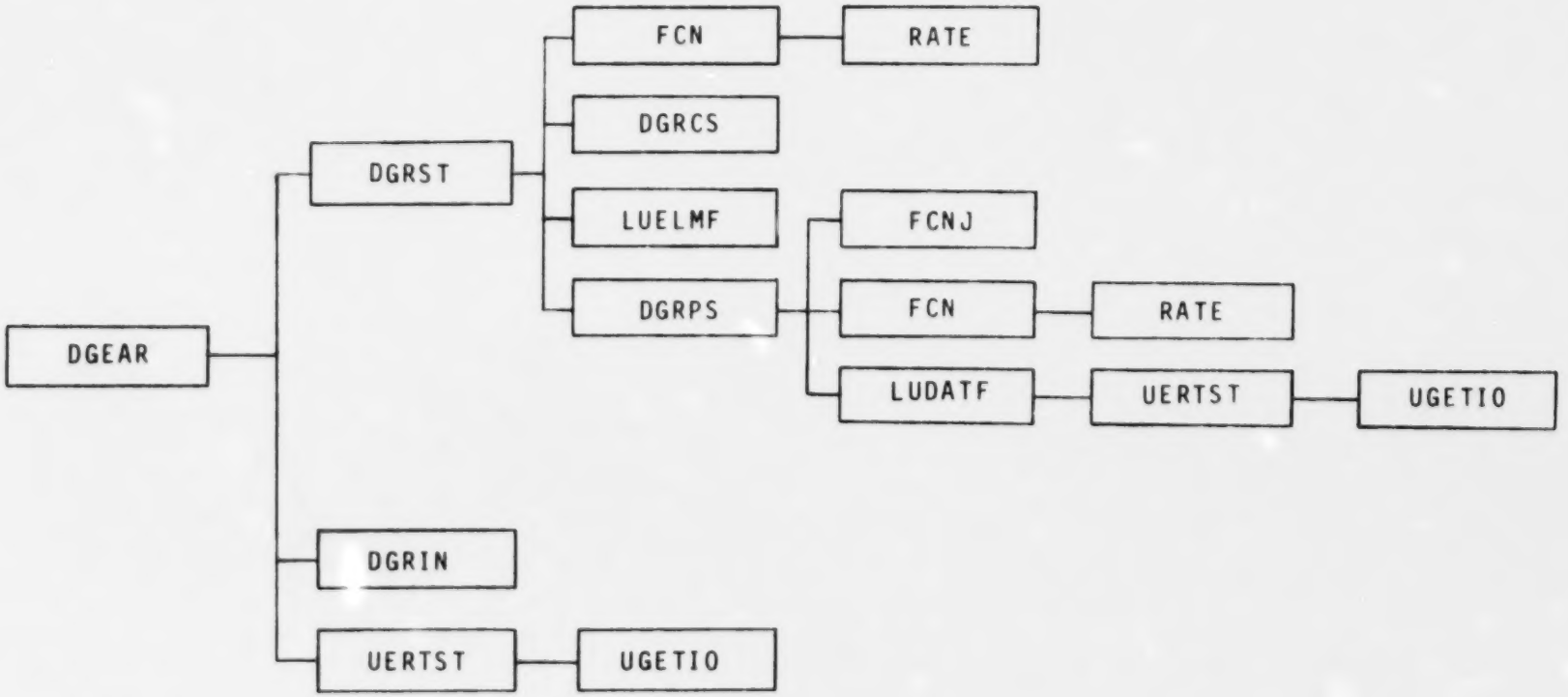


Figure 19 : Simulation Program Organization (cont'd)

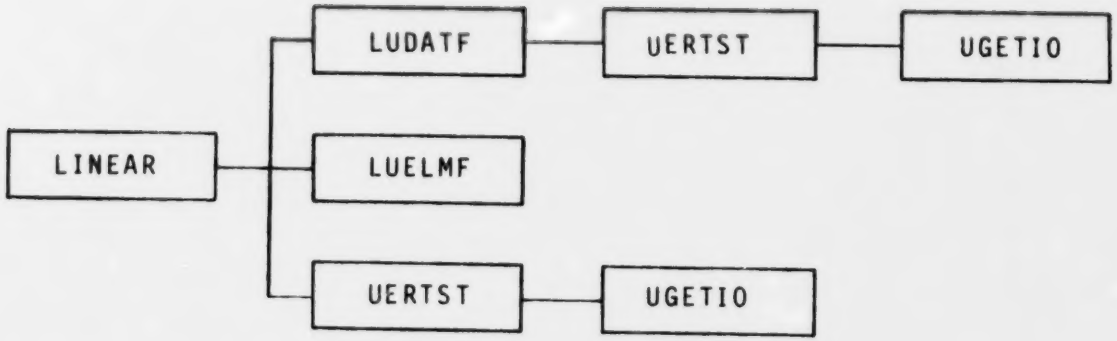
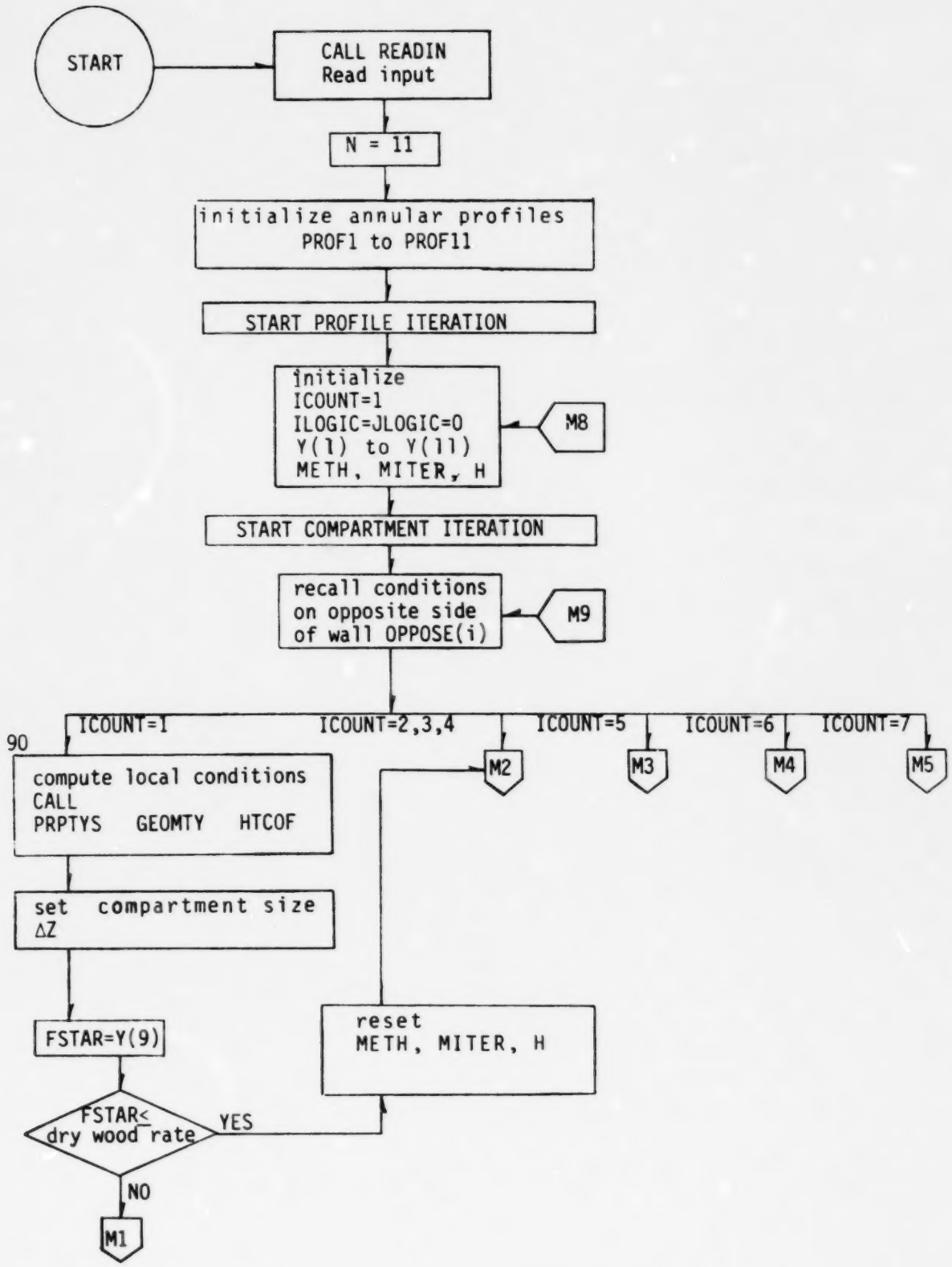
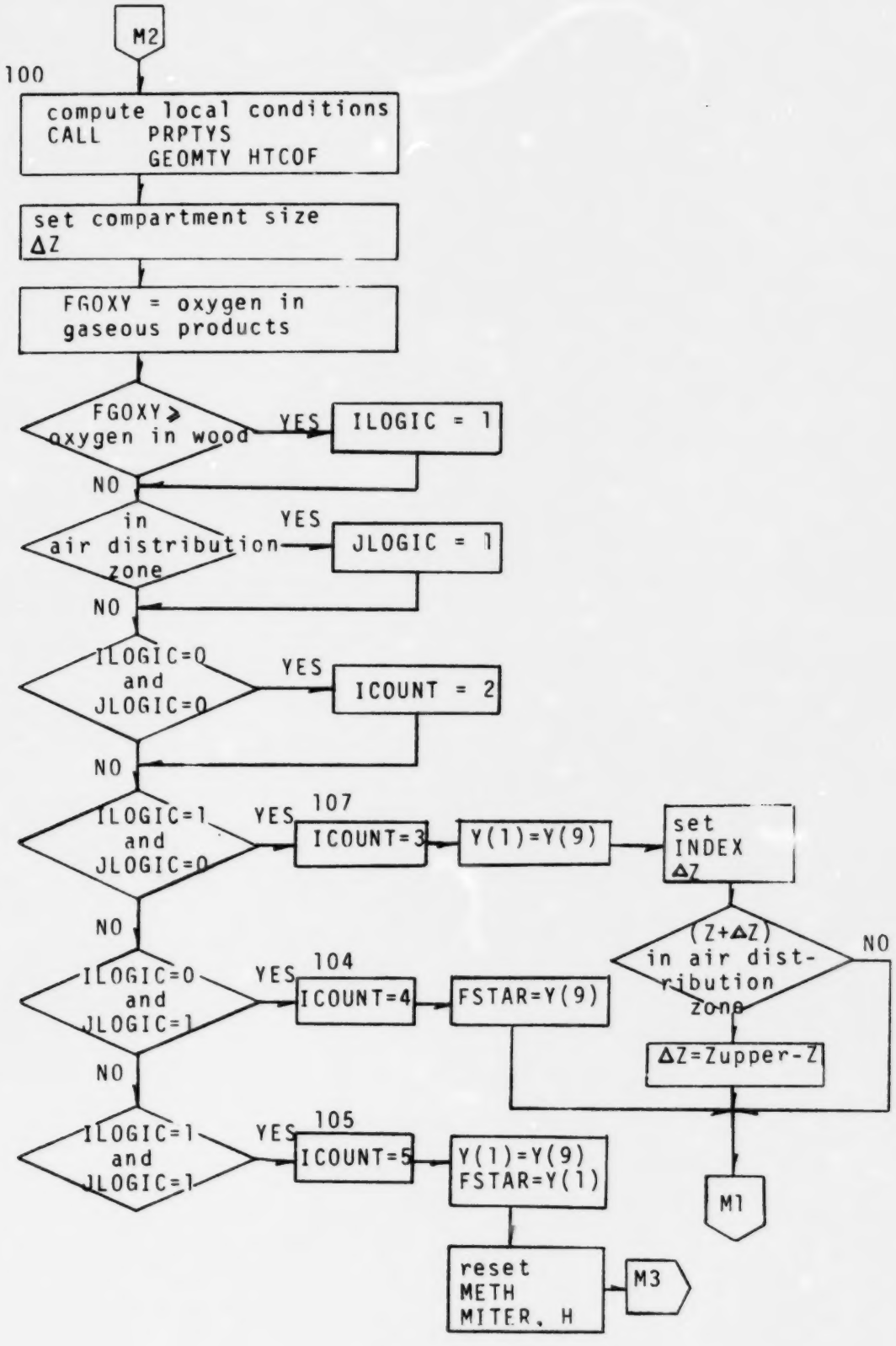


Figure 19 : Simulation Program Organization (cont'd)

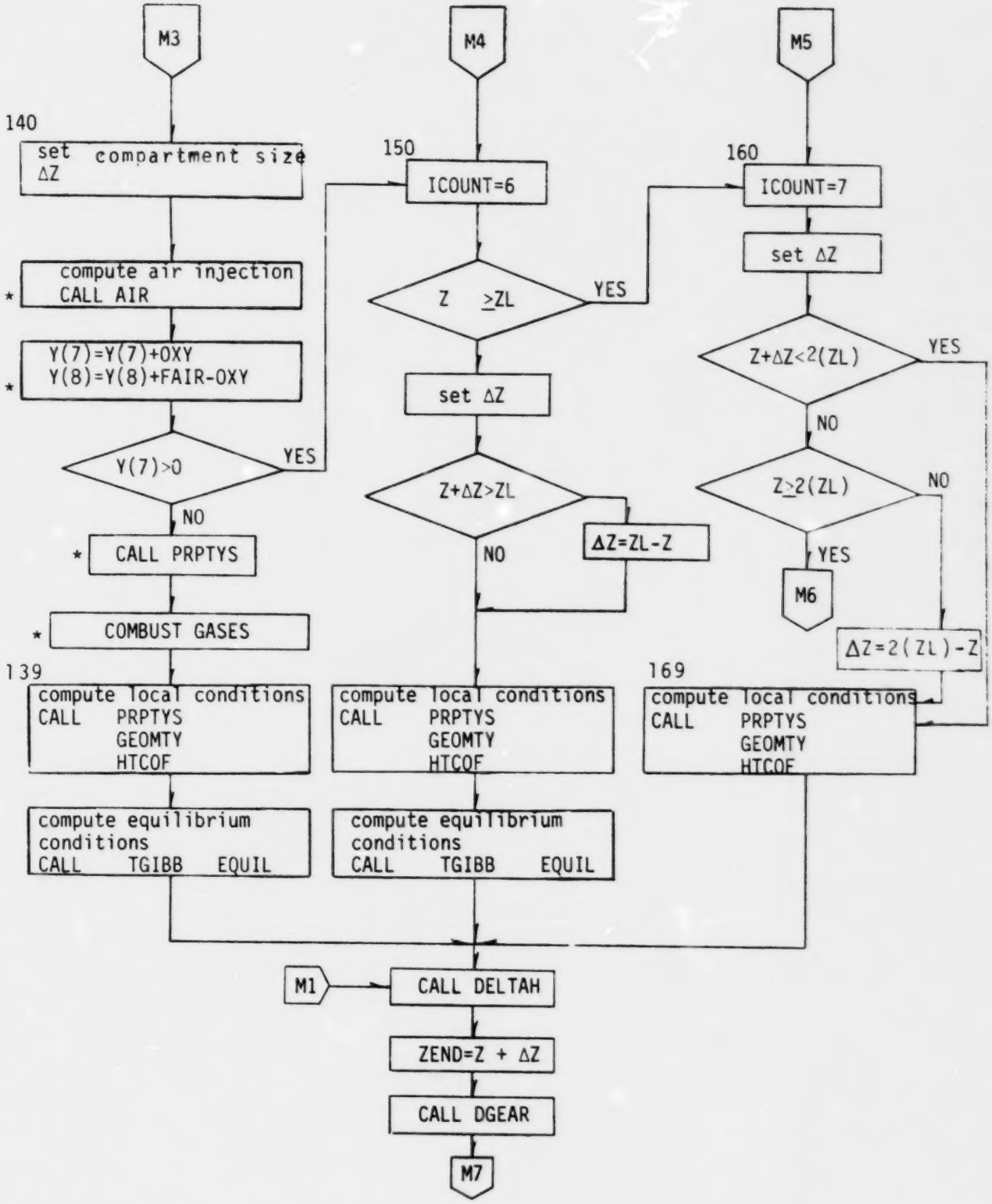
MAIN PROGRAM



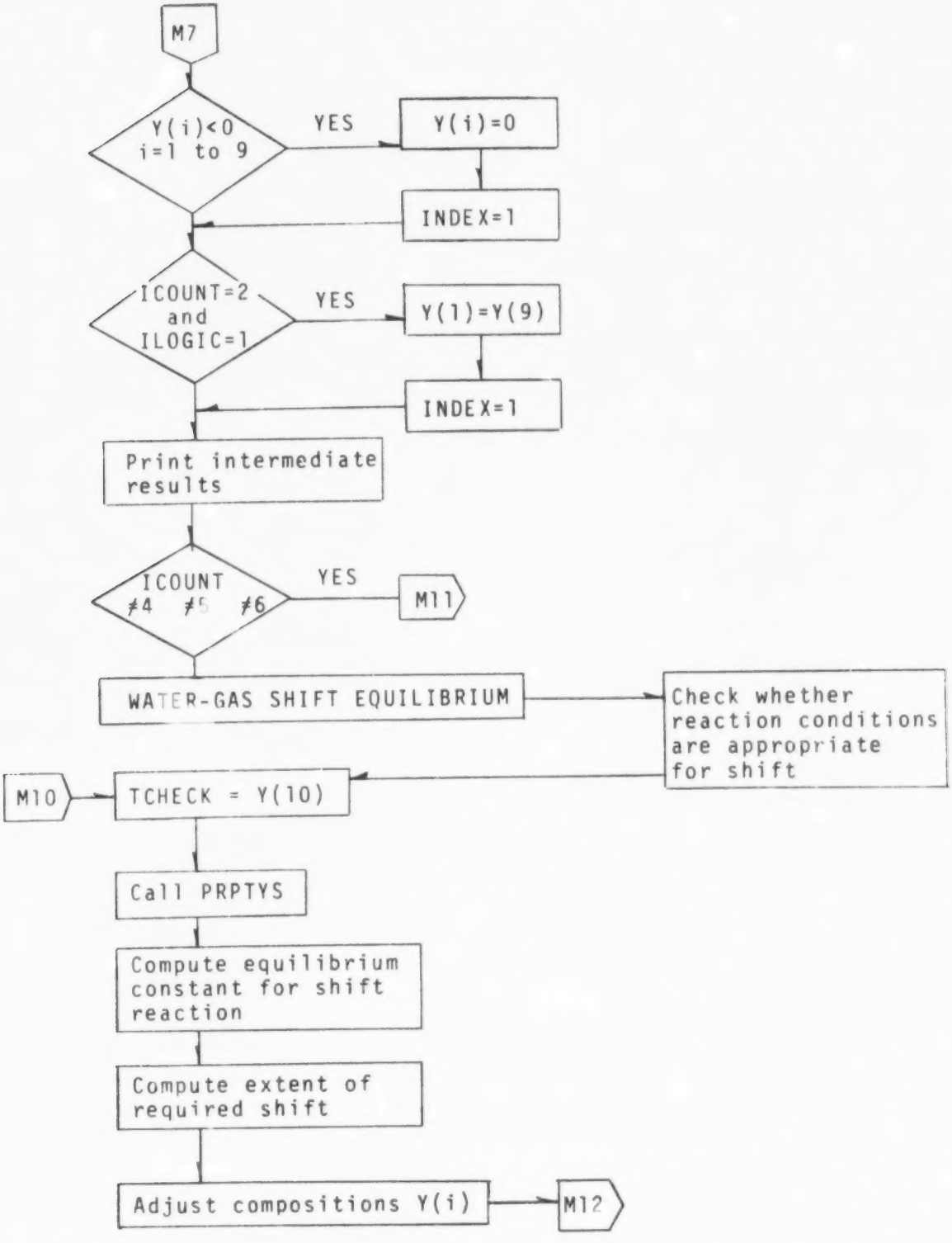
MAIN PROGRAM



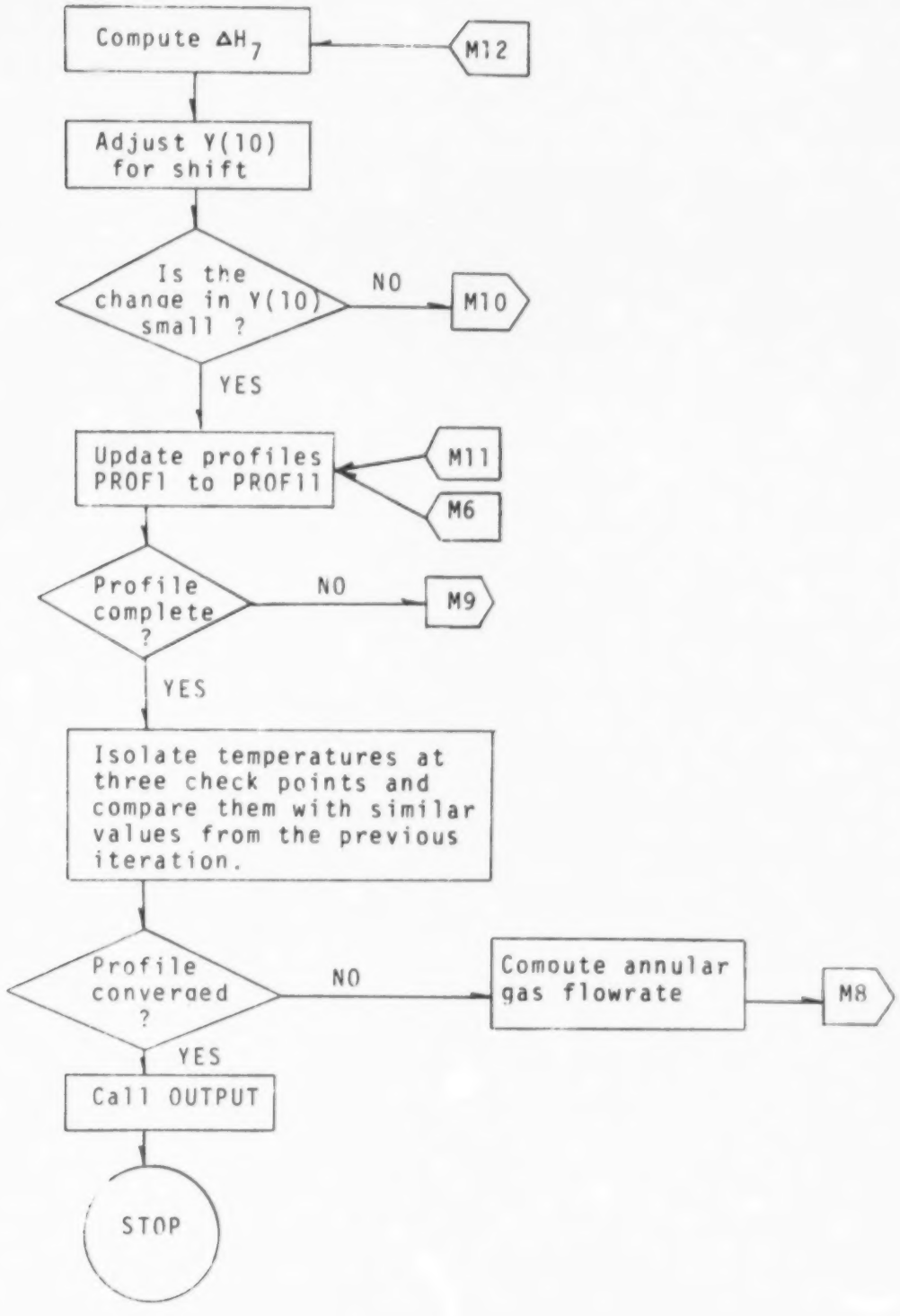
MAIN PROGRAM

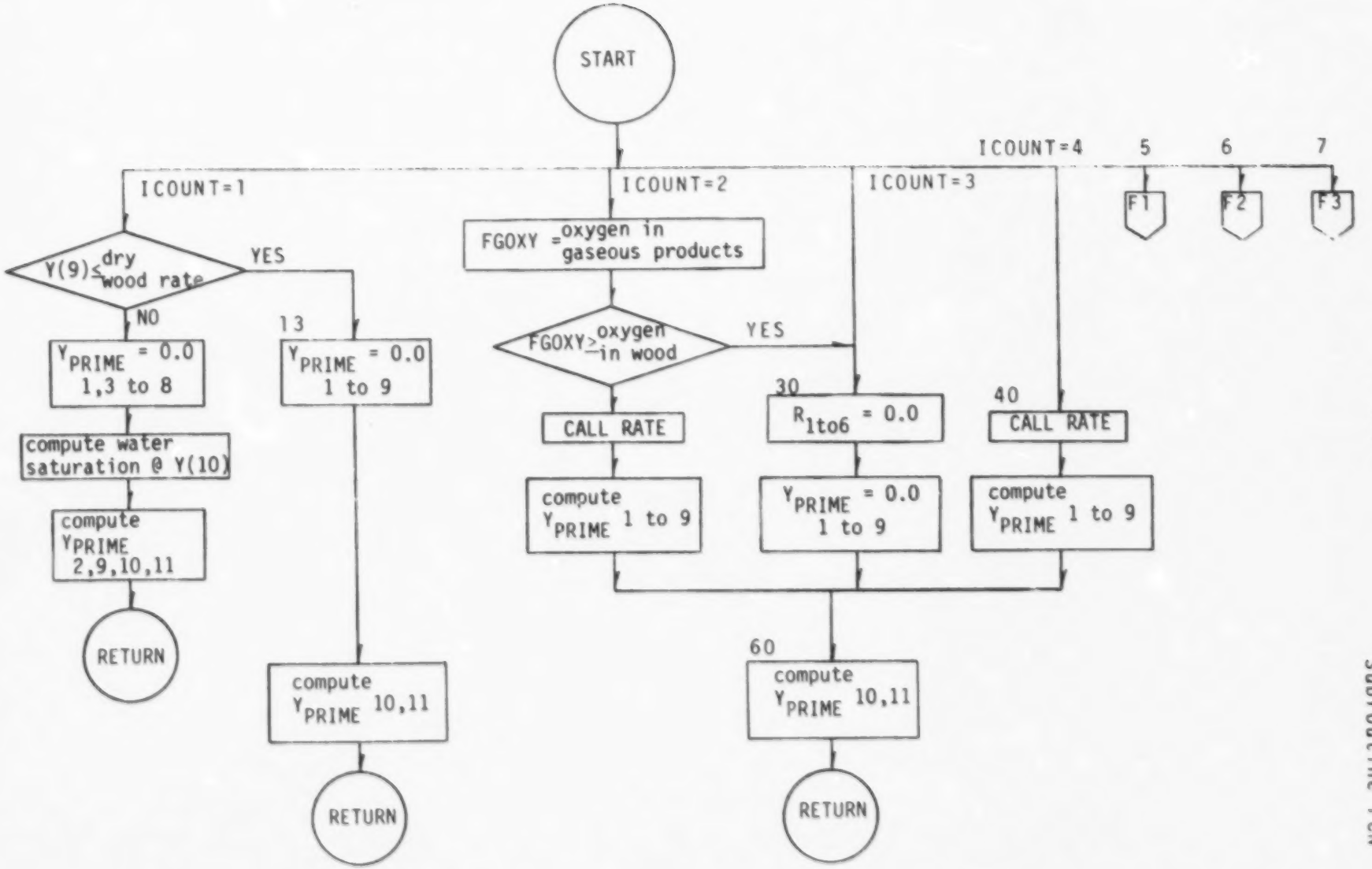


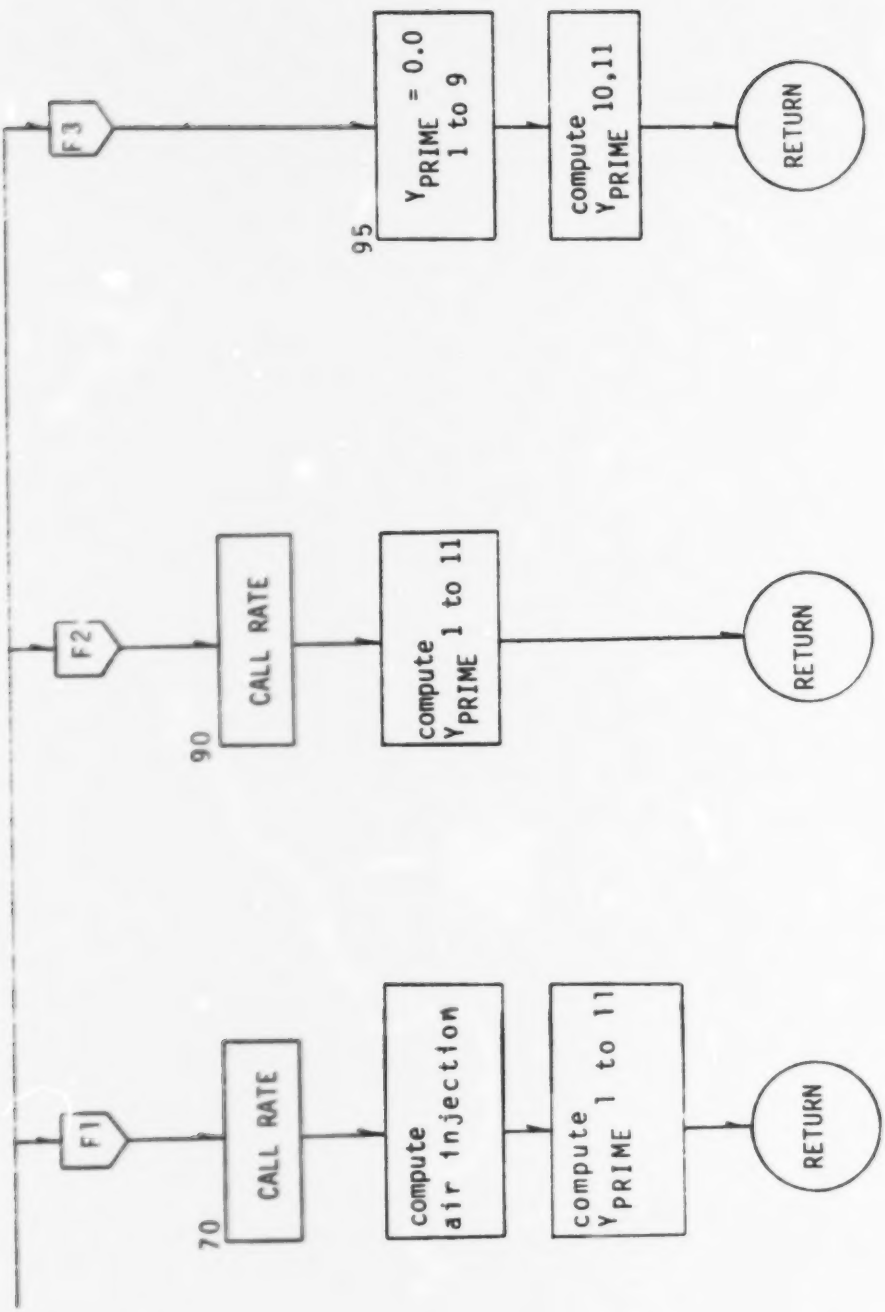
* not in version 83-09.

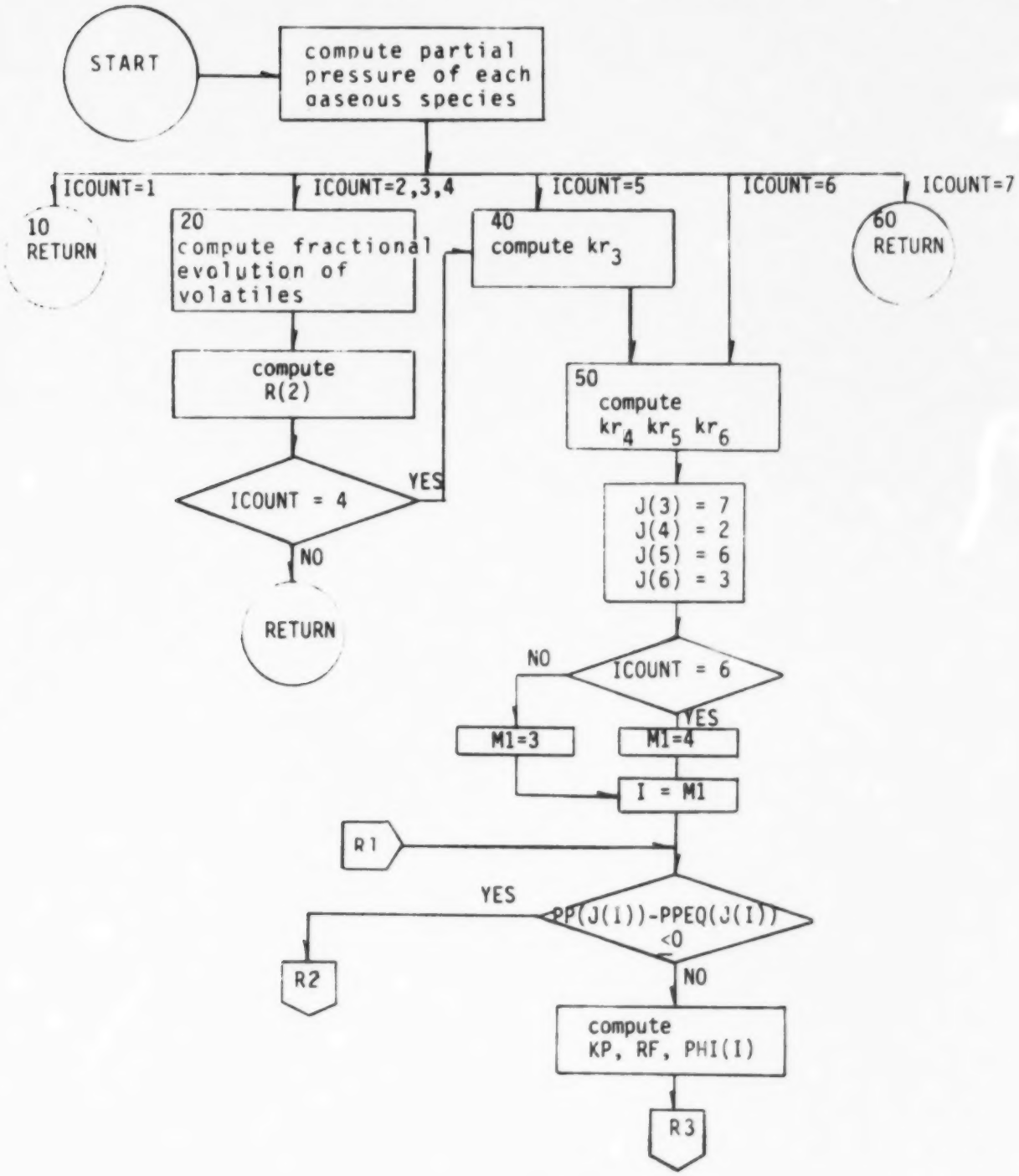

M7
Y(i)<0 i=1 to 9
YES
Y(i)=0
INDEX=1
ICOUNT=2 and ILOGIC=1
YES
Y(1)=Y(9)
INDEX=1
Print intermediate results
ICOUNT ≠4 ≠5 ≠6
YES
M11
WATER-GAS SHIFT EQUILIBRIUM
Check whether reaction conditions are appropriate for shift
M10
TCHECK = Y(10)
Call PRPTYS
Compute equilibrium constant for shift reaction
Compute extent of required shift
Adjust compositions Y(i)
M12

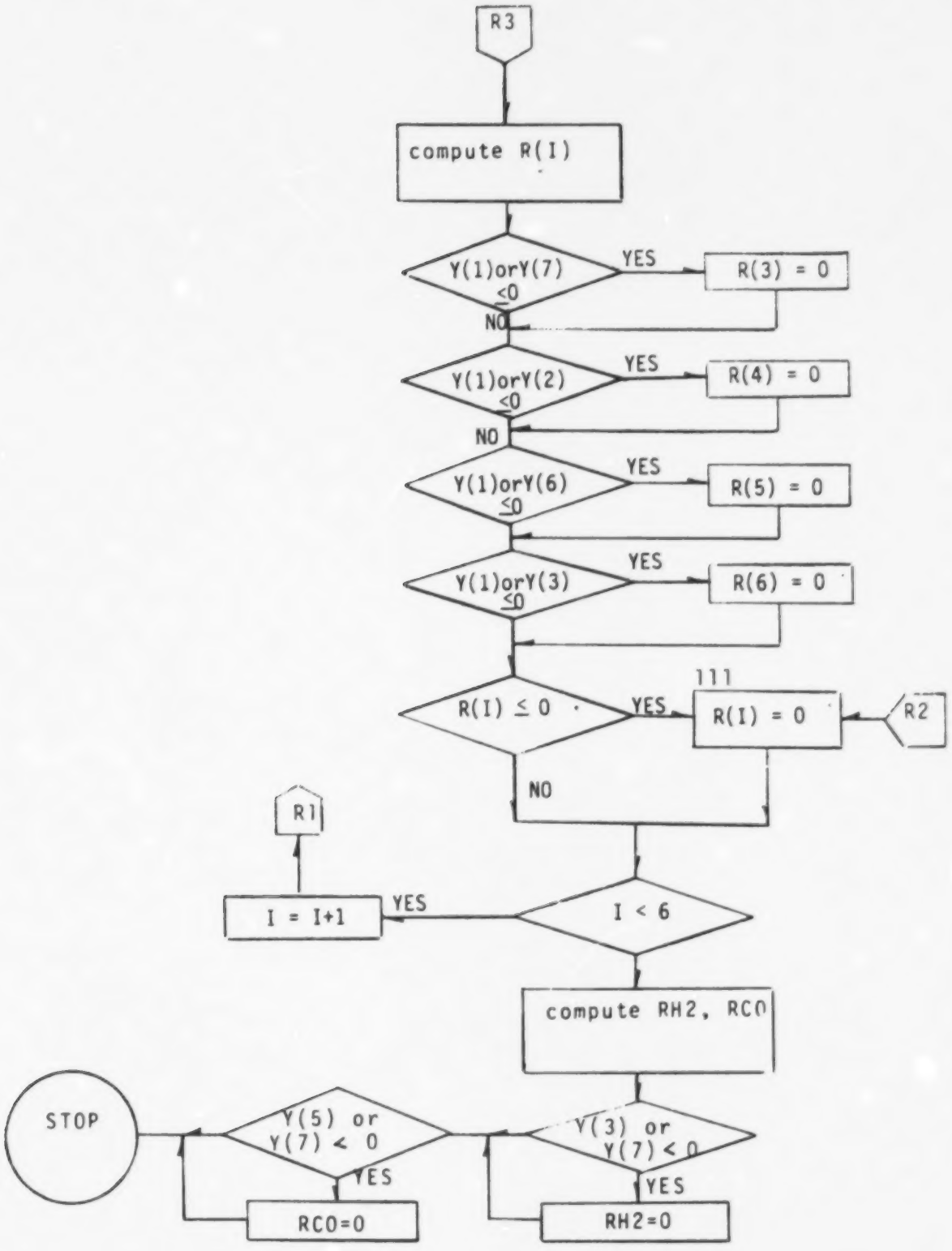
MAIN PROGRAM

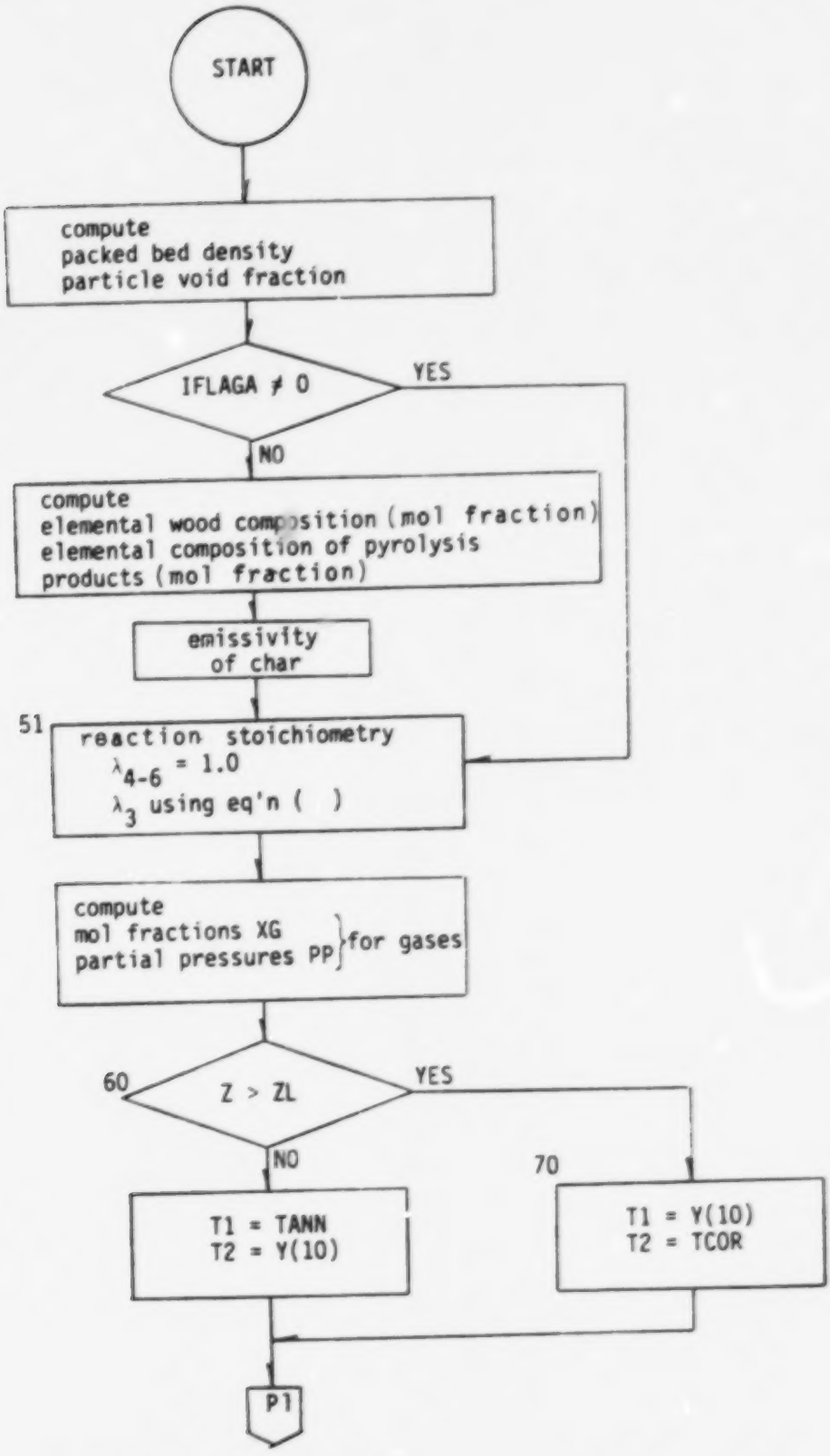


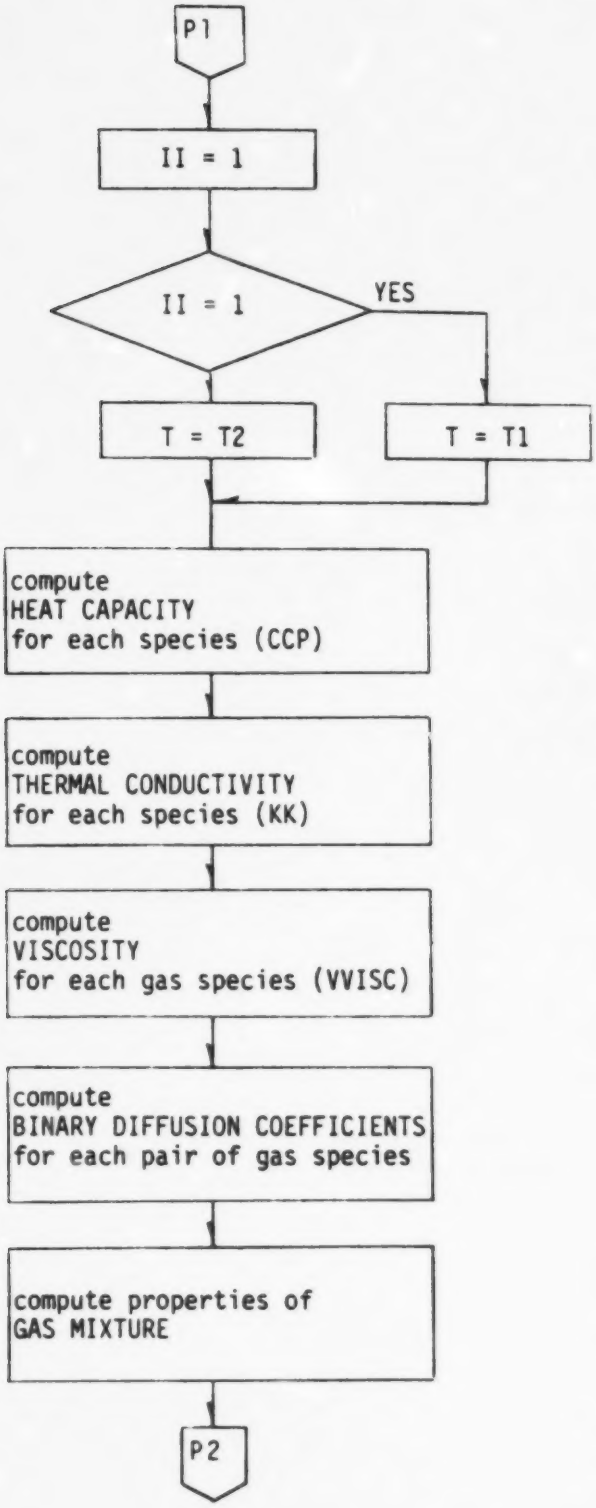

START
ICOUNT=1
ICOUNT=2
ICOUNT=3
ICOUNT=4
5
6
7
F1
F2
F3
Y(9)≤ dry wood rate
YES
NO
13
FGOXY = oxygen in gaseous products
FGOXY≥ oxygen in wood
YES
30
40
60
Y PRIME = 0.0 1,3 to 8
Y PRIME = 0.0 1 to 9
R 1to6 = 0.0
CALL RATE
CALL RATE
compute water saturation @ Y(10)
compute Y PRIME 2,9,10,11
compute Y PRIME 1 to 9
Y PRIME = 0.0 1 to 9
compute Y PRIME 1 to 9
compute Y PRIME 10,11
compute Y PRIME 10,11
RETURN
RETURN
RETURN


F1
70
CALL RATE
compute air injection
compute Y_{PRIME} 1 to 11
RETURN
F2
90
CALL RATE
compute Y_{PRIME} 1 to 11
RETURN
F3
95
Y_{PRIME} = 0.0 1 to 9
compute Y_{PRIME} 10,11
RETURN

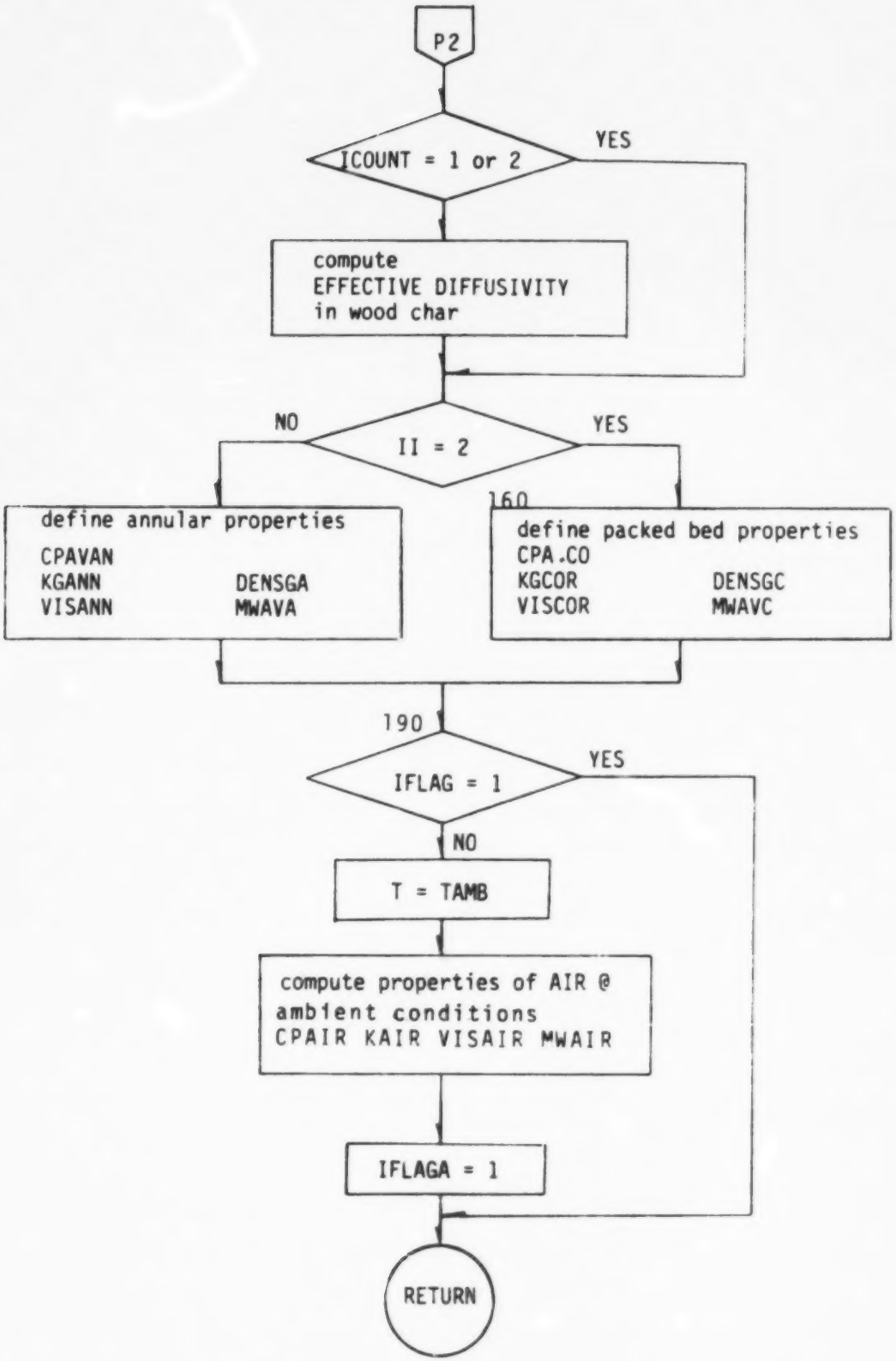

START
compute partial pressure of each gaseous species
ICOUNT=1
ICOUNT=2,3,4
ICOUNT=5
ICOUNT=6
ICOUNT=7
10 RETURN
20 compute fractional evolution of volatiles
40 compute kr_3
60 RETURN
compute R(2)
50 compute kr_4 kr_5 kr_6
ICOUNT = 4
YES
NO
RETURN
J(3) = 7
J(4) = 2
J(5) = 6
J(6) = 3
NO
ICOUNT = 6
YES
M1=3
M1=4
I = M1
R1
YES
PP(J(I))-PPEQ(J(I)) <0
R2
NO
compute KP, RF, PHI(I)
R3


R3
compute R(I)
Y(1)orY(7) ≤0
YES
R(3) = 0
NO
Y(1)orY(2) ≤0
YES
R(4) = 0
NO
Y(1)orY(6) ≤0
YES
R(5) = 0
Y(1)orY(3) ≤0
YES
R(6) = 0
111
R(I) ≤ 0
YES
R(I) = 0
R2
NO
R1
I = I+1
YES
I < 6
compute RH2, RC0
STOP
Y(5) or Y(7) < 0
YES
RC0=0
Y(3) or Y(7) < 0
YES
RH2=0

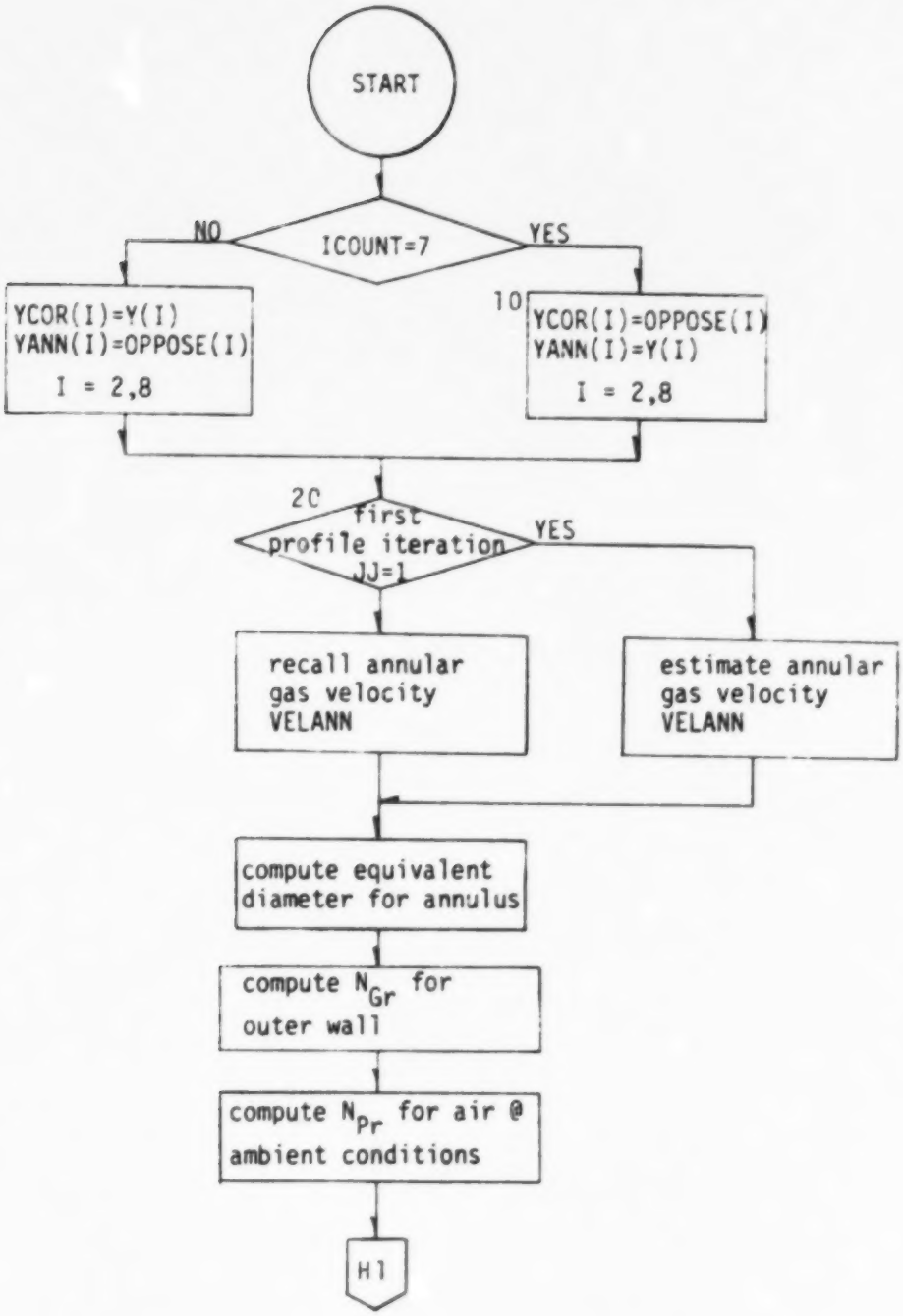

START
compute
packed bed density
particle void fraction
IFLAGA ≠ 0
YES
NO
compute
elemental wood composition (mol fraction)
elemental composition of pyrolysis
products (mol fraction)
emissivity
of char
51
reaction stoichiometry
λ_{4-6} = 1.0
λ_3 using eq'n ( )
compute
mol fractions XG
partial pressures PP
for gases
60
Z > ZL
YES
NO
70
T1 = TANN
T2 = Y(10)
T1 = Y(10)
T2 = TCOR
P1

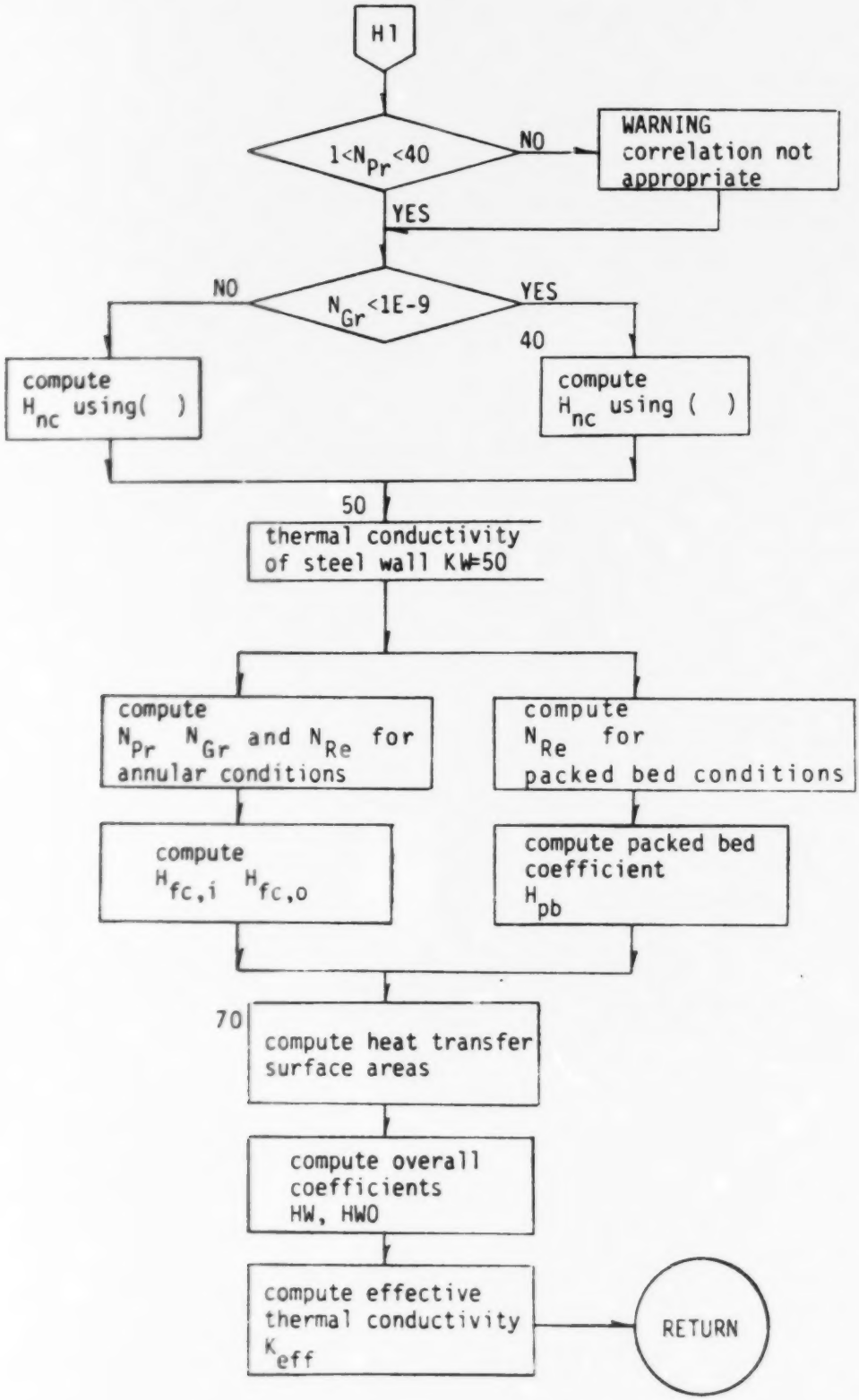

P1
II = 1
II = 1
YES
T = T2
T = T1
compute
HEAT CAPACITY
for each species (CCP)
compute
THERMAL CONDUCTIVITY
for each species (KK)
compute
VISCOSITY
for each gas species (VVISC)
compute
BINARY DIFFUSION COEFFICIENTS
for each pair of gas species
compute properties of
GAS MIXTURE
P2

Subroutine PRPTYS

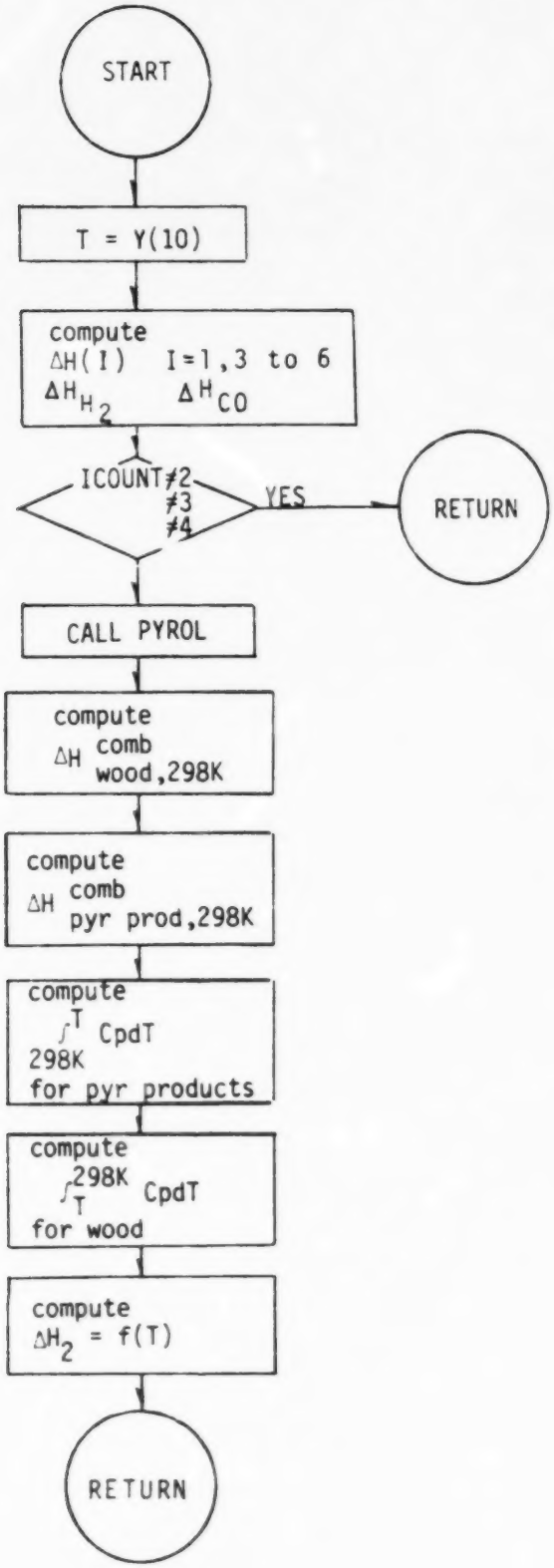


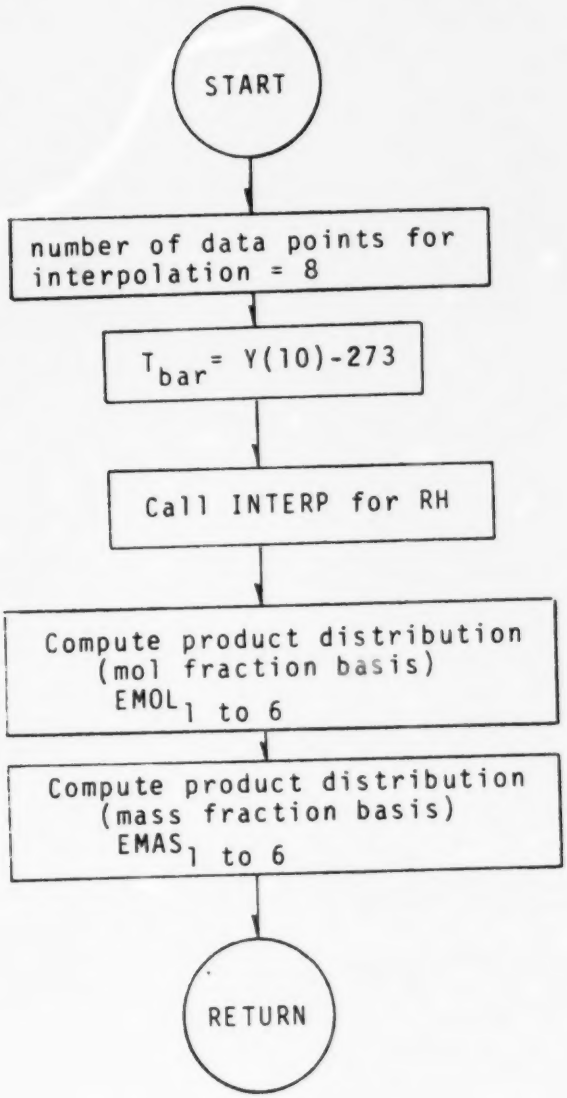
Subroutine HTCOF

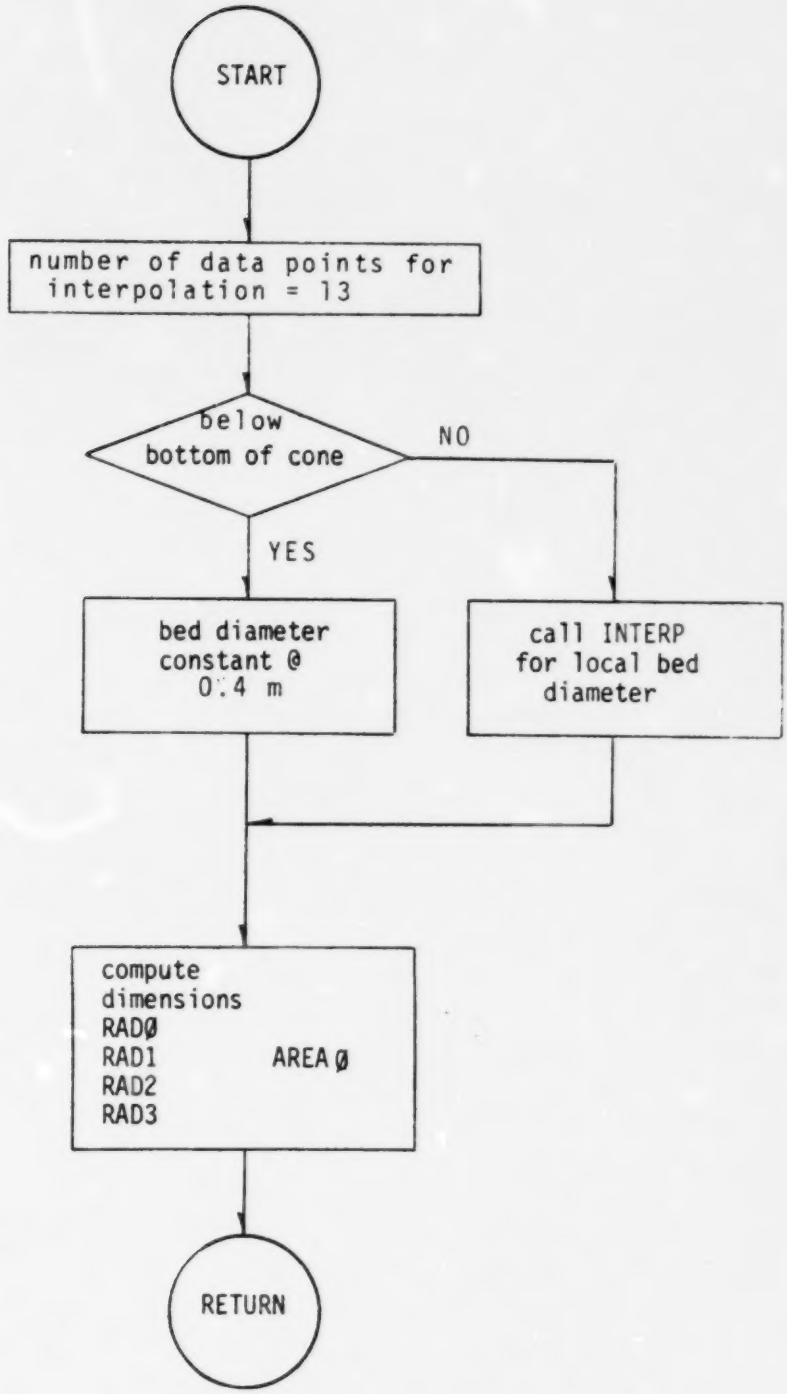


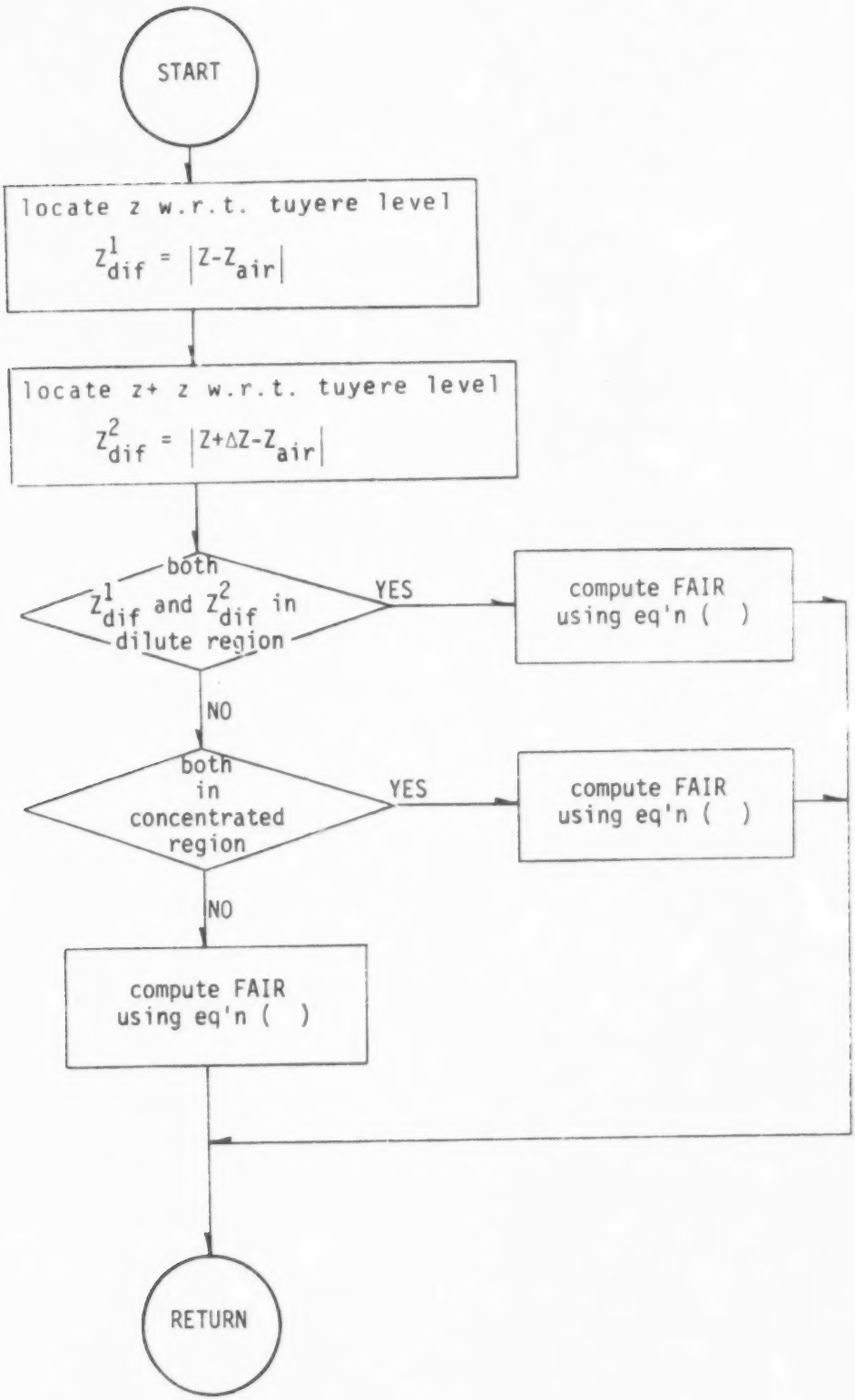

H1
1<N_Pr<40
NO
WARNING correlation not appropriate
YES
NO
N_Gr<1E-9
YES
40
compute H_nc using( )
compute H_nc using ( )
50
thermal conductivity of steel wall KW=50
compute N_Pr N_Gr and N_Re for annular conditions
compute N_Re for packed bed conditions
compute H_fc,i H_fc,o
compute packed bed coefficient H_pb
70
compute heat transfer surface areas
compute overall coefficients HW, HWO
compute effective thermal conductivity K_eff
RETURN

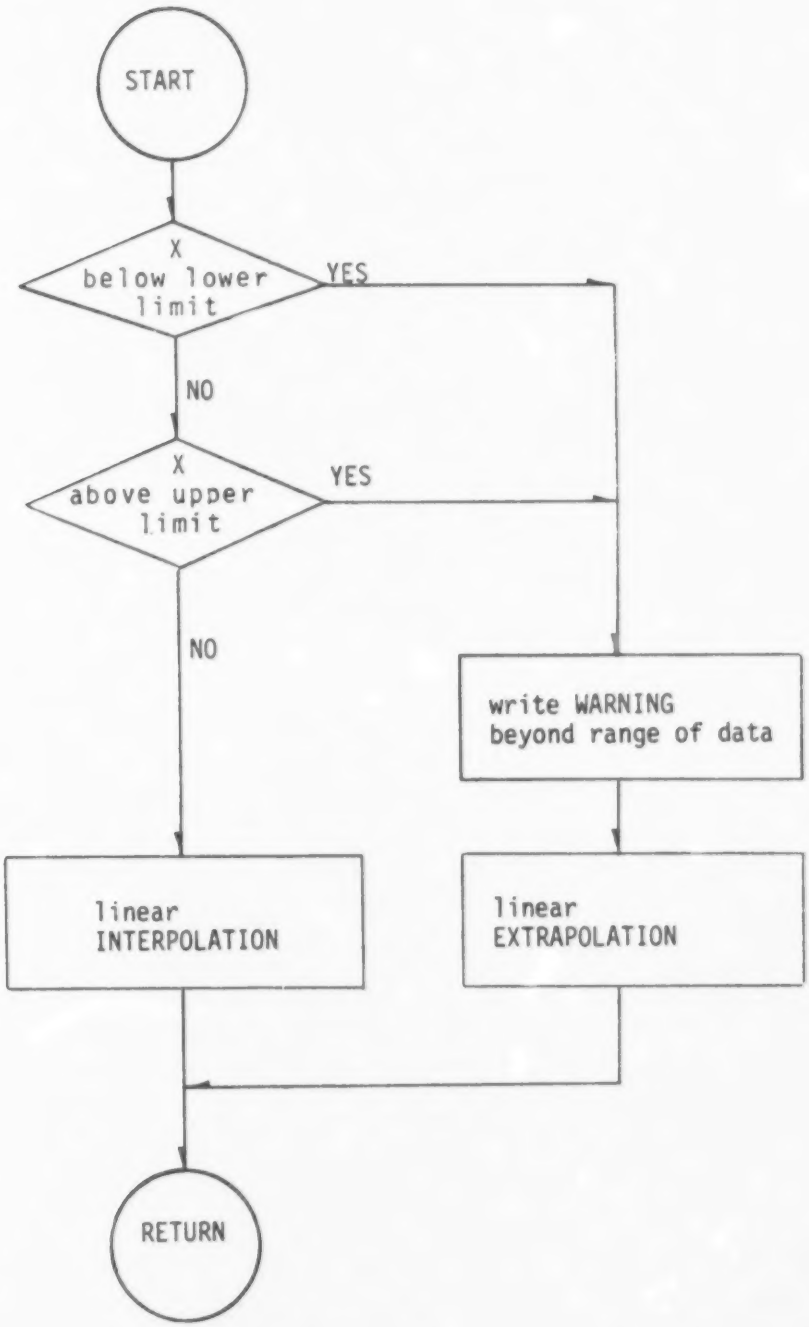
Subroutine DELTAH

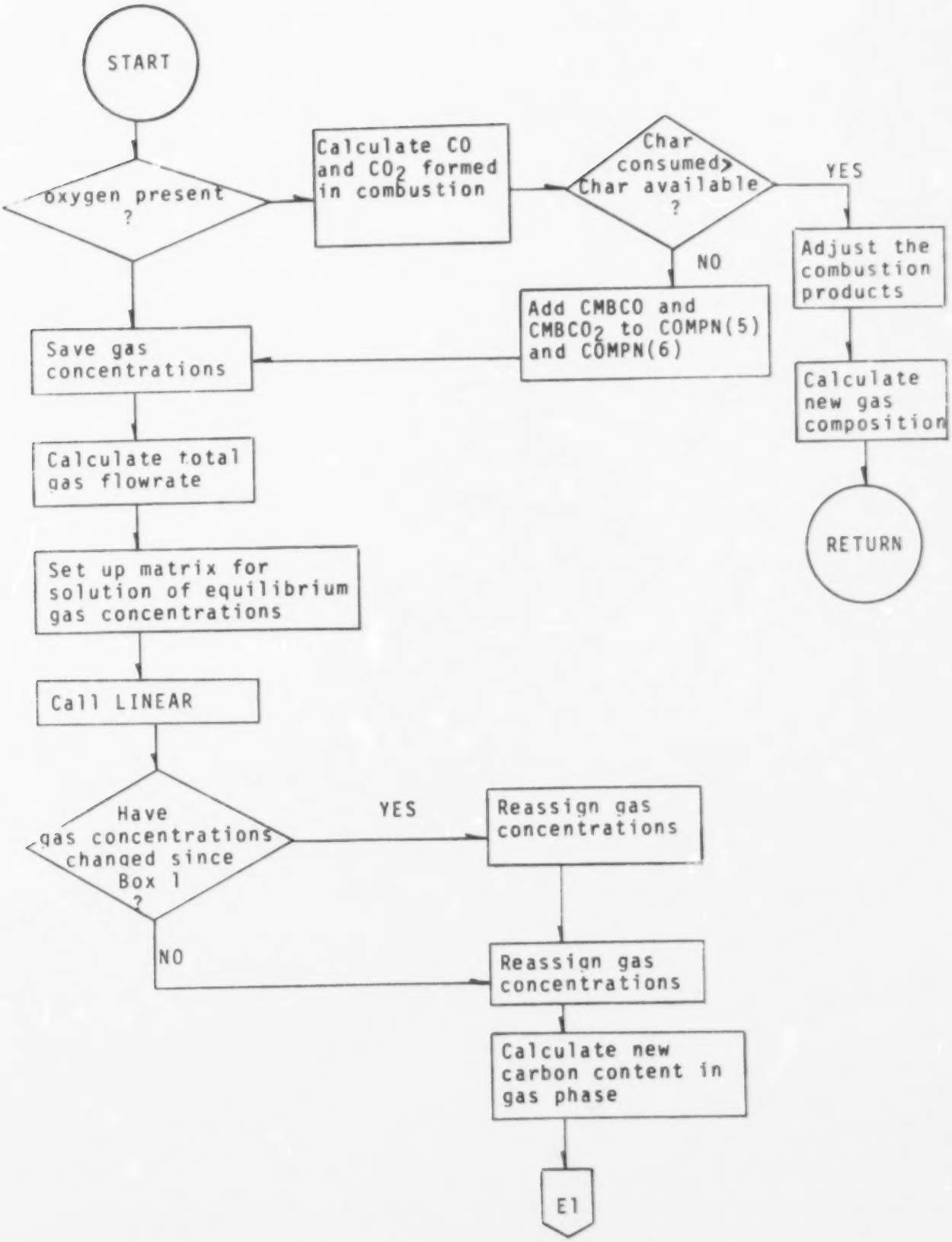


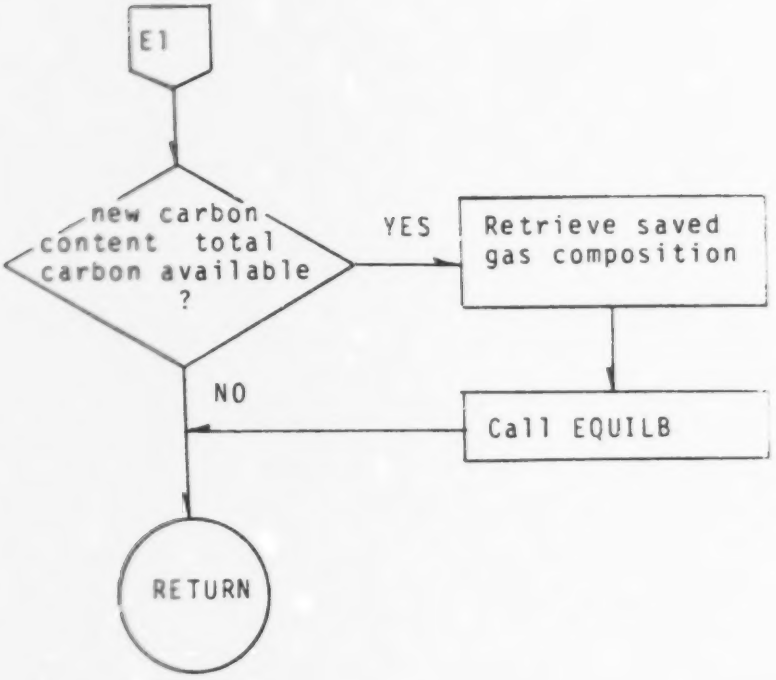

START
number of data points for interpolation = 8
T_{bar} = Y(10)-273
Call INTERP for RH
Compute product distribution (mol fraction basis) $EMOL_{1 \text{ to } 6}$
Compute product distribution (mass fraction basis) $EMAS_{1 \text{ to } 6}$
RETURN

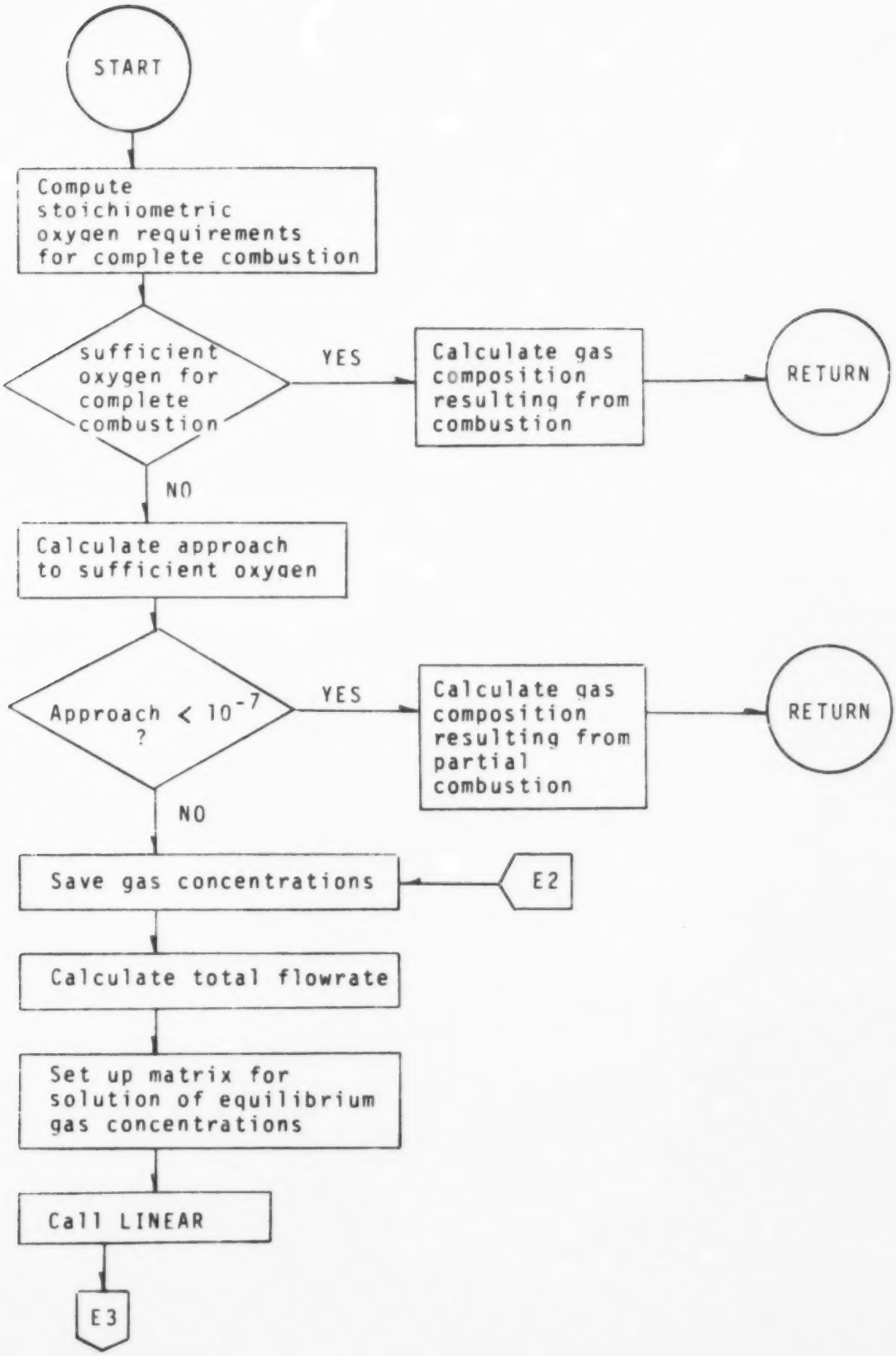

START
number of data points for interpolation = 13
below bottom of cone
NO
YES
bed diameter constant @ 0.4 m
call INTERP for local bed diameter
compute dimensions
RAD0
RAD1
RAD2
RAD3
AREA 0
RETURN

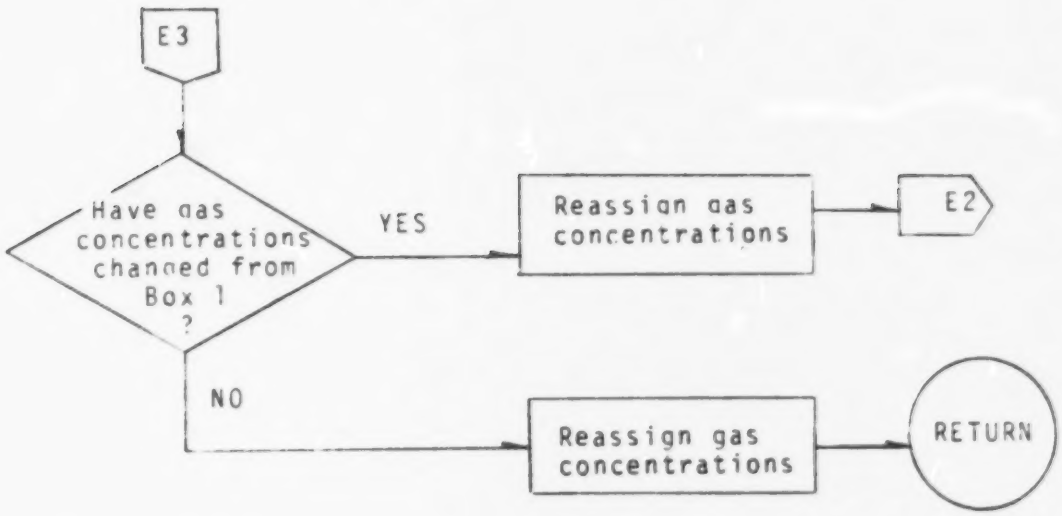

START
locate z w.r.t. tuyere level
$Z^1_{dif} = |Z-Z_{air}|$
locate z+ z w.r.t. tuyere level
$Z^2_{dif} = |Z+\Delta Z-Z_{air}|$
both Z^1_{dif} and Z^2_{dif} in dilute region
YES
compute FAIR using eq'n ( )
NO
both in concentrated region
YES
compute FAIR using eq'n ( )
NO
compute FAIR using eq'n ( )
RETURN

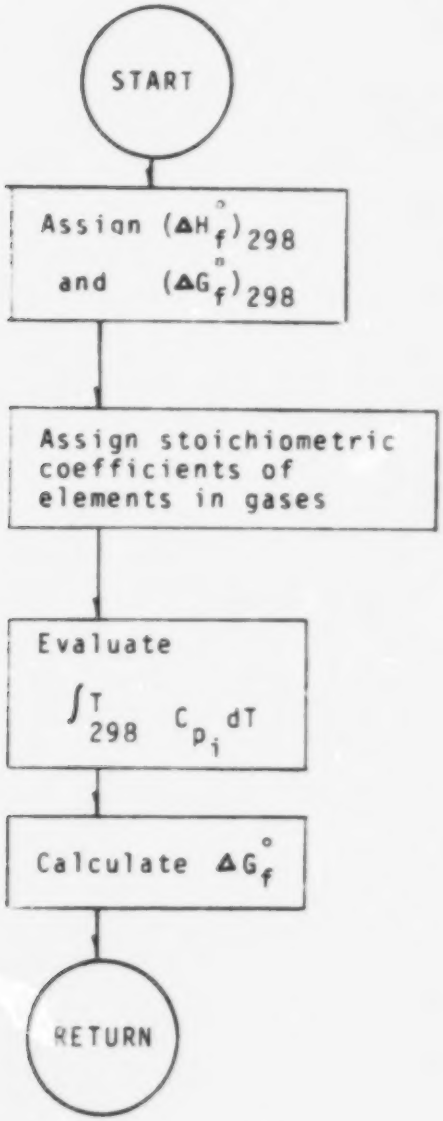

START
X below lower limit
YES
NO
X above upper limit
YES
NO
write WARNING beyond range of data
linear INTERPOLATION
linear EXTRAPOLATION
RETURN


START
oxygen present ?
Calculate CO and CO_2 formed in combustion
Char consumed > Char available ?
YES
NO
Adjust the combustion products
Calculate new gas composition
RETURN
Add CMBCO and $CMBCO_2$ to COMPN(5) and COMPN(6)
Save gas concentrations
Calculate total gas flowrate
Set up matrix for solution of equilibrium gas concentrations
Call LINEAR
Have gas concentrations changed since Box 1 ?
YES
NO
Reassign gas concentrations
Reassign gas concentrations
Calculate new carbon content in gas phase
E1


E1
new carbon content total carbon available ?
YES
Retrieve saved gas composition
NO
Call EQUILB
RETURN


START
Compute stoichiometric oxygen requirements for complete combustion
sufficient oxygen for complete combustion
YES
Calculate gas composition resulting from combustion
RETURN
NO
Calculate approach to sufficient oxygen
Approach < 10^{-7} ?
YES
Calculate gas composition resulting from partial combustion
RETURN
NO
Save gas concentrations
E2
Calculate total flowrate
Set up matrix for solution of equilibrium gas concentrations
Call LINEAR
E3


E3
Have gas concentrations changed from Box 1 ?
YES
Reassign gas concentrations
E2
NO
Reassign gas concentrations
RETURN


START
Assign $(\Delta H_f^\circ)_{298}$ and $(\Delta G_f^\circ)_{298}$
Assign stoichiometric coefficients of elements in gases
Evaluate $\int_{298}^{T} C_{p_i} dT$
Calculate ΔG_f°
RETURN

```
C=======================================================================
C     MAIN PROGRAM
C=======================================================================
C     THIS IS A SIMULATION (VERSION 83-09) OF THE MECHANISTIC
C     MODEL FOR DOWN-DRAFT WOOD GASIFIERS DEVELOPED UNDER ENFOR
C     CONTRACT C-197.  COPIES OF THIS PROGRAM (IN FORTRAN) ARE
C     AVAILABLE FROM :
C           DEPT.OF CHEMICAL ENGINEERING
C           QUEEN'S UNIVERSITY
C           KINGSTON, ONTARIO, CANADA
C           K7L 3N6
C-----------------------------------------------------------------------
C     IFLAGA = 0     FIRST CALL TO PRPTYS
C            = 1     NO MORE NEED TO COMPUTE AMBIENT PROPERTIES
C     IFLAGB = 0     FIRST SOLID TEMPERATURE CALCULATION
C            = 1     NOT FIRST SOLID TEMP CALC
C     IFLAGE = 0     FIRST WATER GAS SHIFT CALCULATION
C            = 1     NOT FIRST WATER GAS SHIFT CALC
C     IFLAGF = 1     IMPOSSIBLE ROOT FOR SHIFT CALC
C     IFLAGG = 1     IMPOSSIBLE ROOT FOR SHIFT CALC
C-----------------------------------------------------------------------
      REAL           YMOL(8),PPQ(8)
      REAL           K7,MOLWT,MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,
     1               LAMBDA,KEFF,KS,Y(11),KR(6),FACTOR(8)
      REAL           PROF1(100),PROF2(100),
     2               PROF3(100),PROF4(100),PROF5(100),PROF6(100),
     3               PROF7(100),PROF8(100),PROF9(100),PROF10(100),
     4               PROF11(100)
      DIMENSION      YY(11),ZETAO(2),DUM(4,2),IWK(11),WK(319)
      COMMON/ANALYS/ANALA,ANALC,ANALH,ANALN,ANALO,PROXW,PROXC,
     1               PROXV,PROXA,PMOLO,PMOLC,PMOLH,EMAS(6),HCOMBW
      COMMON/DIMENS/RAD0,RAD1,RAD2,RAD3,AREA0
      COMMON/GAS    /FAIRIN,EH2O,EO2,EN2,TAIR,PAIR,FAIR,
     1               ZL,ZAIR,WIDTH
      COMMON/INDATA/METH1,METH2,METH3,MITER1,MITER2,MITER3,HH1,HH2,
     1               HH3,TOL,ITERAT
      COMMON/INPUT  /TGUESS,RG,PRESS,TAMB,DP
      COMMON/LOCAL  /IZ,ICOUNT,IFLAGA,JL,JJ,HW,HW0,R(6),RH2,RCO,
     1               DELH(7),DELH2,DELCO,DELTAZ,RECORE,DENSB,DENSP,
     2               FSTAR,TCORS,TCOR,TANN,GIBB(7),H2OSAT,
     3               KEFF,OPPOSE(9),GASFLO
      COMMON/PROFIL/PROF1,PROF2,PROF3,PROF4,PROF5,PROF6,PROF7,
     1               PROF8,PROF9,PROF10
      COMMON/PROPS  /MOLWT(8),MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,
     1               VISANN,VISCOR,VISAIR,CPAVAN,CPANN(8),CPCOR(9),
     2               CPAIR,DIF(8),DEFF(8),LAMBDA(7),EMISS,COMPN(8),
     3               DENSGC,DENSGA,PP(8),PPEQ(8),CPAVCO,KS
      COMMON/WOOD   /FSO,DL,DH,DW,VOIDP,VOID,DENSBO,DENSPO
      COMMON/GEAR   /DUMMY(48),SDUMMY(4),IDUMMY(38)
      EXTERNAL       FCN,FCNJ
      DATA FACTOR/-741.9242,-29.72100,-11.55286,-0.8685635,0.1094098,
     1  0.439993,0.2520658,0.05218684/
      DATA MOLWT    /12.01115,18.0152,2.01580,16.0428,28.0106,44.0100,
```

```
     1              31.9988,28.0134/
C-----------------------------------------------------------------
      CALL ASSIGN (5,'DY1:INPUT.DAT',0,'RDO')
C     CALL ASSIGN (8,'DY1:OUT.DAT',0,'OLD')
      CALL ASSIGN (6,'TT:',0)
      CALL ASSIGN (7,'LP:',0)
C-----------------------------------------------------------------
C     INITIALIZE VARIABLES
      CALL READIN
      CALL CLOSE(5)
      IFLAGA=0
      FAIR=0.0
      DP=(6.*DL*DH*DW/3.1416)**0.33333333
      VOID=(DENSPO-DENSBO)/DENSPO
      ZUPPER=ZAIR-WIDTH
      N=11
      INDEX=1
      DUMX2=IZ
      DO 20 IK=1,IZ
      DUMX1=IK
      PROF11(IK)=2.*ZL*DUMX1/DUMX2
 20   CONTINUE
      SUMH=0.0
      DO 21 IO=1,8
      SUMH=SUMH+FACTOR(IO)*(0.65-0.01*(TAMB-273.15))**(IO-1)
 21   CONTINUE
      H2OSAT=220.88*EXP(0.010/TAMB*(374.136-(TAMB-273.))*SUMH)
     1       *0.9869
      AMB=1.+H2OSAT
      AMBH2O=H2OSAT/AMB
      AMBN2=0.79/AMB
      AMBO2=0.21/AMB
      GVOID=FSO/DENSPO*VOID/(1.-VOID)*PRESS/TAMB/8.205E-5
C-----INITIALIZE ANNULAR CONDITIONS ----------------------------
      DO 41 I1=IZ/2+1,IZ
      PROF1(I1) =0.0
      PROF2(I1) =0.038
      PROF3(I1) =0.004
      PROF4(I1) =0.002
      PROF5(I1) =0.056
      PROF6(I1) =0.060
      PROF7(I1) =0.000
      PROF8(I1) =0.140
      PROF9(I1) =0.000
      DUMX3=I1
      DUMX=(DUMX3-DUMX2/2.)/(DUMX2/2.)
      PROF10(I1)=1173.-500.*DUMX
 41   CONTINUE
      DO 42 I2=1,IZ/2
      PROF11(I2)=0.0
 42   CONTINUE
 60   CONTINUE
C-----PROFILE ITERATION ----------------------------------------
```

```
      DO 440 JJ=1,ITERAT
      ICOUNT=1
      ILOGIC=0
      JLOGIC=0
      METH=METH1
      MITER=MITER1
      H=HH1
      DO 70 JK=2,7
      Y(JK)=0.0
 70   CONTINUE
      Y(1)=FSO/(1.+PROXW)*(PROXC+PROXA)
      Y(2)=GVOID*AMBH2O*MOLWT(2)/1000.
      Y(7)=GVOID*AMBO2 *MOLWT(7)/1000.
      Y(8)=GVOID*AMBN2 *MOLWT(8)/1000.
      Y(9)=FSO
      Y(10)=TGUESS
      Y(11)=1.0
      Z=0.0
      ZEND=0.0
C-----COMPARTMENT ITERATION ----------------------------------------
      DO 380 JL=1,IZ
      ZCALC=2.*ZL-Z
      CALL INTERP(IZ,PROF11,PROF1,OPPOSE(1),ZCALC)
      CALL INTERP(IZ,PROF11,PROF2,OPPOSE(2),ZCALC)
      CALL INTERP(IZ,PROF11,PROF3,OPPOSE(3),ZCALC)
      CALL INTERP(IZ,PROF11,PROF4,OPPOSE(4),ZCALC)
      CALL INTERP(IZ,PROF11,PROF5,OPPOSE(5),ZCALC)
      CALL INTERP(IZ,PROF11,PROF6,OPPOSE(6),ZCALC)
      CALL INTERP(IZ,PROF11,PROF7,OPPOSE(7),ZCALC)
      CALL INTERP(IZ,PROF11,PROF8,OPPOSE(8),ZCALC)
      CALL INTERP(IZ,PROF11,PROF9,OPPOSE(9),ZCALC)
      IF(ICOUNT.EQ.7)GO TO 1003
      CALL INTERP(IZ,PROF11,PROF10,TANN,ZCALC)
      TCOR=Y(10)
      GO TO 1004
 1003 CALL INTERP(IZ,PROF11,PROF10,TCOR,ZCALC)
      TANN=Y(10)
 1004 DENSB=DENSBO*Y(9)/FSO
      DENSP=DENSPO*Y(9)/FSO
      GO TO(90,100,100,100,140,150,160),ICOUNT
C-----DRYING ZONE ---------------------------------------------------
 90   CALL PRPTYS(Y)
      CALL GEOMTY(Z)
      CALL HTCOF(Y)
      CALL RATE(Y)
      DELTAZ=0.08
      IF(Z.GE.0.65)DELTAZ=0.02
      FSTAR=Y(9)
      IF(Y(9).GT.FSO/(1.+PROXW))GO TO 170
      METH=METH2
      MITER=MITER2
      H=HH2
C-----PYROLYSIS ZONE ------------------------------------------------
```

```
  100  CALL PRPTYS(Y)
       CALL GEOMTY(Z)
       CALL HTCOF(Y)
       DELTAZ=0.01
       FGOXY=((Y(2)-FSO*PROXW/(1.+PROXW))/MOLWT(2)+Y(5)/MOLWT(5)+
      1       2.*Y(6)/MOLWT(6))*15.9994
       IF(FGOXY.GE.(FSO/(1.+PROXW)*ANALO))ILOGIC=1
       IF((ZEND+DELTAZ-ZUPPER).GE.0.0)JLOGIC=1
       IF(ILOGIC.EQ.0.AND.JLOGIC.EQ.0)ICOUNT=2
       IF(ILOGIC.EQ.1.AND.JLOGIC.EQ.0)GO TO 107
       IF(ILOGIC.EQ.0.AND.JLOGIC.EQ.1)GO TO 104
       IF(ILOGIC.EQ.1.AND.JLOGIC.EQ.1)GO TO 105
       GO TO 170
  104  ICOUNT=4
       FSTAR=Y(9)
       GO TO 170
  105  ICOUNT=5
       Y(1)=Y(9)
       FSTAR=Y(1)
       METH=METH3
       MITER=MITER3
       H=HH3
       GO TO 140
  107  ICOUNT=3
       Y(1)=Y(9)
       INDEX=1
       DELTAZ=0.005
       IF((ZEND+DELTAZ).GT.ZUPPER)DELTAZ=ZUPPER-ZEND
       GO TO 170
C-----COMBUSTION ZONE ----------------------------------------------
  140  DELTAZ=0.005
       IF((Z.GT.ZAIR+WIDTH).AND.(Y(7).LE.0.0))GO TO 150
C      CALL AIR(Z)
C      IF(FAIR.LE.0.1E-10)FAIR=0.0
C      OXY=FAIR/MWAIR*MOLWT(7)*0.21
C      Y(7)=Y(7)+OXY
C      Y(8)=Y(8)+(FAIR-OXY)
C      Y(2)=Y(2)
C      INDEX=1
C      IF(Y(7).GT.0.1E-10)GO TO 139
C      Y(7)=0.000
C      GO TO 150
  139  CALL PRPTYS(Y)
       CALL GEOMTY(Z)
       CALL HTCOF(Y)
       CALL TGIBB(Y)
       CALL EQUIL(Y)
       GO TO 170
C-----GASIFICATION ZONE ---------------------------------------------
  150  ICOUNT=6
       IF(Z.GE.ZL)GO TO 160
       DELTAZ=0.01
       IF((Z+DELTAZ).GT.ZL)DELTAZ=ZL-Z
```

```
      CALL PRPTYS(Y)
      CALL GEOMTY(Z)
      CALL HTCOF(Y)
      CALL TGIBB(Y)
      CALL EQUIL(Y)
      GO TO 170
C-----ANNULUS ----------------------------------------------------------
 160  ICOUNT=7
      DELTAZ=0.05
      IF((Z+DELTAZ).LT.(2.*ZL))GO TO 169
      IF(Z.GE.(2.*ZL))GO TO 360
      DELTAZ=(2.*ZL)-Z
 169  CALL PRPTYS(Y)
      CALL GEOMTY(Z)
      CALL HTCOF(Y)
 170  CALL DELTAH(Y)
      ZEND=ZEND+DELTAZ
C-------------------------------------------------------------------------
 175  CALL DGEAR(N,FCN,FCNJ,Z,H,Y,ZEND,TOL,METH,MITER,INDEX,IWK,
     1           WK,IER)
C-------------------------------------------------------------------------
 712  CONTINUE
      DO 174 IV=1,9
      IF(Y(IV).LT.1.E-7)GO TO 173
 174  CONTINUE
      GO TO 172
 173  DO 171 IVV=1,9
      IF(Y(IVV).LT.1.E-7)Y(IVV)=0.0
 171  CONTINUE
      INDEX=1
 172  IF(ICOUNT.EQ.7)GO TO 177
      IF((ICOUNT.EQ.2).AND.(ILOGIC.EQ.1))GO TO 776
      GO TO 778
 776  Y(1)=Y(9)
      INDEX=1
 778  WRITE(7,179)ICOUNT,JL,Z,TANN,FAIR
C     AAX=AX/Y(11)
C     WRITE(7,1833)AAX,AX,BX,CX,DX
C     WRITE(7,1838)KR(3),KR(4),KR(5),KR(6)
C     WRITE(7,1844)R(3),R(4),R(5),R(6),RH2,RCO
C     WRITE(7,1848)DELH(3),DELH(4),DELH(5),DELH(6),DELH2,DELCO
C     WRITE(7,1854)EMAS(1),EMAS(2),EMAS(3),EMAS(4),EMAS(5),EMAS(6)
C     WRITE(7,1855)PP(2),PP(3),PP(4),PP(5),PP(6),PP(7)
C     WRITE(7,1866)PPEQ(2),PPEQ(3),PPEQ(4),PPEQ(5),PPEQ(6),PPEQ(7)
      GO TO 178
 177  WRITE(7,179)ICOUNT,JL,Z,TCOR
C     WRITE(7,1833)AAX,AX,BX,CX,DX
 178  WRITE(7,181)Y(1),Y(2),Y(3),Y(4),Y(5)
      WRITE(7,1822)Y(6),Y(7),Y(8),Y(9),Y(10),Y(11)
 179  FORMAT(/,1X,I1,1X,I2,1X,F4.2,2X,G10.3,2X,G10.3)
 181  FORMAT(1X,5(G10.3,2X))
 1822 FORMAT(1X,5(G10.3,2X),G10.3,/)
C1833 FORMAT(1X,'AABCD ',5(1X,G10.3))
```

```
C1838 FORMAT(1X,'KR     ',4(1X,G10.3))
C1844 FORMAT(1X,'RATES ',6(1X,G10.3))
C1848 FORMAT(1X,'DELH  ',6(1X,G10.3))
C1854 FORMAT(1X,'EMAS  ',6(1X,G10.3))
C1855 FORMAT(1X,'PP    ',6(1X,G10.3))
C1866 FORMAT(1X,'PPEQ  ',6(1X,G10.3))
      IF((ICOUNT.NE.6).AND.(ICOUNT.NE.5).AND.(ICOUNT.NE.4))GO TO 360
C-----ADJUST FOR WATER-GAS SHIFT EQUILIBRIUM --------------------
 182  CONTINUE
      IF((Y(3).LE.0.).OR.(Y(5).LE.0.))GO TO 360
      IF(Y(10).LT.750.)GO TO 360
      DO 185 IL=1,10
      YY(IL)=Y(IL)
 185  CONTINUE
 180  TCHECK=YY(10)
      CALL PRPTYS(YY)
      K7=EXP(1.510*ALOG(YY(10))-0.141E-3*YY(10)-0.460E5/YY(10)**2
     1      +5697./YY(10)-15.604)
      ALPHA1=K7-1.0
      ALPHA2=-(K7*(COMPN(5)+COMPN(2))+COMPN(6)+COMPN(3))
      ALPHA3=K7*COMPN(5)*COMPN(2)-COMPN(6)*COMPN(3)
      ALPHA4=(ALPHA2**2.-4.*ALPHA1*ALPHA3)**0.5
      ZETA0(1)=(-ALPHA2+ALPHA4)/2./ALPHA1
      ZETA0(2)=(-ALPHA2-ALPHA4)/2./ALPHA1
C     CHECK FOR CORRECT ROOT
      DO 200 IS=1,2
      DUM(1,IS)=COMPN(2)-ZETA0(IS)
      DUM(2,IS)=COMPN(3)+ZETA0(IS)
      DUM(3,IS)=COMPN(5)-ZETA0(IS)
      DUM(4,IS)=COMPN(6)+ZETA0(IS)
 200  CONTINUE
      IFLAGF=0
      DO 210 IT=1,4
      IF(DUM(IT,1).LT.0.)IFLAGF=1
 210  CONTINUE
      IFLAGG=0
      DO 220 IU=1,4
      IF(DUM(IU,2).LT.0.)IFLAGG=1
 220  CONTINUE
      IF(IFLAGF.EQ.1.AND.IFLAGG.EQ.1)GO TO 230
      IF(IFLAGF.EQ.1)GO TO 240
      IX=1
      GO TO 260
 230  WRITE(6,235)
 235  FORMAT(5X,'BOTH ZETA ROOTS BAD')
      WRITE(6,221)IFLAGF,IFLAGG
 221  FORMAT(' IFLAGFG',2X,I1,2X,I1)
      STOP
 240  IX=2
 260  ZETA=ZETA0(IX)
      YY(2)=(COMPN(2)-ZETA)*MOLWT(2)/1000.
      YY(3)=(COMPN(3)+ZETA)*MOLWT(3)/1000.
```

```
      YY(5)=(COMPN(5)-ZETA)*MOLWT(5)/1000.
      YY(6)=(COMPN(6)+ZETA)*MOLWT(6)/1000.
      DELH(7)=(3.00*YY(10)-0.28E-3*YY(10)**2.+1.83E5/YY(10)
     1       -11320.23)*4.184
      YY(10)=YY(10)-ZETA*DELH(7)/(YY(1)*CPCOR(1)+1000.*
     1        (YY(2)*CPCOR(2)/MOLWT(2)+YY(3)*CPCOR(3)/MOLWT(3)
     2        +YY(4)*CPCOR(4)/MOLWT(4)+YY(5)*CPCOR(5)/MOLWT(5)
     3        +YY(6)*CPCOR(6)/MOLWT(6)+YY(7)*CPCOR(7)/MOLWT(7)
     4        +YY(8)*CPCOR(8)/MOLWT(8)))
      INDEX=1
      IF(YY(10).LT.0.999*TCHECK.OR.YY(10).GT.1.001*TCHECK)GO TO 180
      DO 270 IV=1,10
      Y(IV)=YY(IV)
  270 CONTINUE
      WRITE(7,1444)Y(2),Y(3),Y(5),Y(6),Y(10)
 1444 FORMAT(1X,'SHIFT ',5(1X,G10.3))
C-----CHECK CONVERGENCE OF PROFILE-------------------------------
  360 CONTINUE
      PROF1(JL)=Y(1)
      PROF2(JL)=Y(2)
      PROF3(JL)=Y(3)
      PROF4(JL)=Y(4)
      PROF5(JL)=Y(5)
      PROF6(JL)=Y(6)
      PROF7(JL)=Y(7)
      PROF8(JL)=Y(8)
      PROF9(JL)=Y(9)
      PROF10(JL)=Y(10)
      PROF11(JL)=Z
  380 CONTINUE
      DO 390 JL=1,IZ
      TMAX=AMAX1(PROF10(JL))
  390 CONTINUE
      IF(JJ.EQ.1)GO TO 435
  400 IF(ABS(TMAX-TMAXO).GT.1.)GO TO 440
  410 IF((PROF10(IZ/2)-XXBOTO).GT.1.)GO TO 440
  420 IF((PROF10(IZ)  -XXTOPO).GT.1.)GO TO 440
  430 IF((PROF10(20)  -XXMIDO).GT.1.)GO TO 440
      GO TO 450
  435 TMAXO=TMAX
      XXBOTO=PROF10(IZ/2)
      XXTOPO=PROF10(IZ)
      XXMIDO=PROF10(20)
      GASFLO=(Y(2)/MOLWT(2)+Y(3)/MOLWT(3)+Y(4)/MOLWT(4)+Y(5)/MOLWT(5)
     1    +Y(6)/MOLWT(6)+Y(7)/MOLWT(7)+Y(8)/MOLWT(8))*1000.
  440 CONTINUE
C-----SEND CONVERGED PROFILE TO OUTPUT FILE----------------------
  450 CALL OUTPUT
      STOP
      END
```

```
C=======================================================================
      SUBROUTINE FCN(N,Z,Y,YPRIME)
C=======================================================================
C     THIS SUBROUTINE CONTAINS THE DIFFERENTIAL EQUATIONS THAT
C     REPRESENT THE MASS AND ENERGY BALANCES AT EACH POINT IN
C     THE GASIFIER.
C-----------------------------------------------------------------------
      REAL           MWAVA,MWAVC,MWAIR,MOLWT,KGANN,KGCOR,KAIR,
     1               LAMBDA,YPRIME(11),Y(11),KEFF,KS
      REAL           WK(319),FACTOR(8)
      INTEGER        IDUMMY(38)
      COMMON/GEAR   /DUMMY(48),SDUMMY(4),IDUMMY
      COMMON/ANALYS/ANALA,ANALC,ANALH,ANALN,ANALO,PROXW,PROXC,
     1               PROXV,PROXA,PMOLO,PMOLC,PMOLH,EMAS(6),HCOMBW
      COMMON/DIMENS/RAD0,RAD1,RAD2,RAD3,AREA0
      COMMON/GAS    /FAIRIN,EH20,EO2,EN2,TAIR,PAIR,FAIR,ZL,
     1               ZAIR,WIDTH
      COMMON/INPUT  /TGUESS,RG,PRESS,TAMB,DP
      COMMON/LOCAL  /IZ,ICOUNT,IFLAGA,JL,JJ,HW,HWO,R(6),RH2,RCO,
     1               DELH(7),DELH2,DELCO,DELTAZ,RECORE,DENSB,DENSP,
     2               FSTAR,TCORS,TCOR,TANN,GIBB(7),H2OSAT,
     3               KEFF,OPPOSE(9),GASFLO
      COMMON/PROPS  /MOLWT(8),MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,
     1               VISANN,VISCOR,VISAIR,CPAVAN,CPANN(8),CPCOR(9),
     2               CPAIR,DIF(8),DEFF(8),LAMBDA(7),EMISS,COMPN(8),
     3               DENSGC,DENSGA,PP(8),PPEQ(8),CPAVCO,KS
      COMMON/WOOD   /FSO,DL,DH,DW,VOIDP,VOID,DENSBO,DENSPO
      DATA FACTOR/-741.9242,-29.72100,-11.55286,-0.8685635,0.1094098,
     1  0.439993,0.2520658,0.05218684/
      GO TO (10,20,30,40,70,90,95),ICOUNT
C-----DRYING ZONE ----------------------------------------------------
   10 IF(Y(9).LE.FSO/(1.+PROXW))GO TO 13
      YPRIME(1)=0.0
      YPRIME(3)=0.0
      YPRIME(4)=0.0
      YPRIME(5)=0.0
      YPRIME(6)=0.0
      YPRIME(7)=0.0
      YPRIME(8)=0.0
      U=6.47/Y(10)-0.01
      V=0.0
      DO 11 I=1,8
      V=V+FACTOR(I)*(3.38-0.01*Y(10))**(I-1)
   11 CONTINUE
      UPRIME=-6.47/(Y(10)**2)
      VPRIME=-0.01*FACTOR(2)
      DO 12 II=3,8
      VPRIME=VPRIME-((II-1)*0.01*FACTOR(II)*(3.38-0.01*Y(10))**(II-2))
   12 CONTINUE
C
      PPRIME=217.99*(U*VPRIME+V*UPRIME)*EXP(U*V)
      YPRIME(10)=Y(11)
      YPRIME(11)=((Y(9)*CPCOR(9)+1000.*(Y(2)*CPCOR(2)/MOLWT(2)
```

```
     1           +Y(3)*CPCOR(3)/MOLWT(3)+Y(4)*CPCOR(4)/MOLWT(4)
     2           +Y(5)*CPCOR(5)/MOLWT(5)+Y(6)*CPCOR(6)/MOLWT(6)
     3           +Y(7)*CPCOR(7)/MOLWT(7)+Y(8)*CPCOR(8)/MOLWT(8))
     4           +DELH(1)*Y(8)*MOLWT(2)/MOLWT(8)/PRESS*PPRIME)*Y(11)
     5           -2.*3.1416*RADO*HW*(TANN-Y(10)))/KEFF/AREAO
      YPRIME(2)=Y(8)*MOLWT(2)/MOLWT(8)/PRESS*PPRIME*YPRIME(10)
      YPRIME(9)=-YPRIME(2)
C     AX=(Y(9)*CPCOR(9)+1000.*(Y(2)*CPCOR(2)/MOLWT(2)+Y(3)*CPCOR(3)
C    1   /MOLWT(3)+Y(4)*CPCOR(4)/MOLWT(4)+Y(5)*CPCOR(5)/MOLWT(5)
C    2   +Y(6)*CPCOR(6)/MOLWT(6)+Y(7)*CPCOR(7)/MOLWT(7)+
C    3   Y(8)*CPCOR(8)/MOLWT(8)))*Y(11)
C     BX=+DELH(1)*Y(8)*MOLWT(2)/MOLWT(8)/PRESS*PPRIME*Y(11)
C     CX=-2.*3.1416*RADO*HW*(TANN-Y(10))
C     DX=KEFF*AREAO
      RETURN
 13   DO 14 II=1,9
      YPRIME(II)=0.0
 14   CONTINUE
      YPRIME(10)=Y(11)
      YPRIME(11)=((Y(9)*CPCOR(9)+1000.*(Y(2)*CPCOR(2)/MOLWT(2)
     1           +Y(3)*CPCOR(3)/MOLWT(3)+Y(4)*CPCOR(4)/MOLWT(4)
     2           +Y(5)*CPCOR(5)/MOLWT(5)+Y(6)*CPCOR(6)/MOLWT(6)
     3           +Y(7)*CPCOR(7)/MOLWT(7)+Y(8)*CPCOR(8)/MOLWT(8)))
     4           *Y(11)
     5           -2.*3.1416*RADO*HW*(TANN-Y(10)))/KEFF/AREAO
C     AX=(Y(9)*CPCOR(9)+1000.*(Y(2)*CPCOR(2)/MOLWT(2)+Y(3)*CPCOR(3)
C    1   /MOLWT(3)+Y(4)*CPCOR(4)/MOLWT(4)+Y(5)*CPCOR(5)/MOLWT(5)
C    2   +Y(6)*CPCOR(6)/MOLWT(6)+Y(7)*CPCOR(7)/MOLWT(7)+
C    3   Y(8)*CPCOR(8)/MOLWT(8)))*Y(11)
C     BX=0.0
C     CX=-2.*3.1416*RADO*HW*(TANN-Y(10))
C     DX=KEFF*AREAO
      RETURN
C-----PYROLYSIS ZONE -------------------------------------------
 20   FGOXY=((Y(2)-FSO*PROXW/(1.+PROXW))/MOLWT(2)+Y(5)/MOLWT(5)
     1      +2.*Y(6)/MOLWT(6))*15.9994
      IF(FGOXY.GE.(FSO/(1.+PROXW)*ANALO))GO TO 30
      CALL RATE(Y)
      YPRIME(9)=-R(2)*AREAO
      YPRIME(1)=0.
      YPRIME(2)=R(2)*EMAS(2)*AREAO
      YPRIME(3)=R(2)*EMAS(3)*AREAO
      YPRIME(4)=R(2)*EMAS(4)*AREAO
      YPRIME(5)=R(2)*EMAS(5)*AREAO
      YPRIME(6)=R(2)*EMAS(6)*AREAO
      YPRIME(7)=0.0
      YPRIME(8)=0.0
      GO TO 60
C-----VOLATILES ALL EVOLVED BUT NOT YET COMBUSTION --------------
 30   CONTINUE
      DO 31 IG=1,6
      R(IG)=0.000
 31   CONTINUE
```

```
      DO 25 IH=1,9
      YPRIME(IH)=0.000
 25   CONTINUE
      GO TO 60
C-----COMBINED PYROLYSIS AND COMBUSTION -------------------------
 40   CALL RATE(Y)
C     EMASM=1.-EMAS(1)
C     YPRIME(1)=R(2)*EMAS(1)/EMASM*AREA0
C    1    -(LAMBDA(3)*R(3)+R(4)+R(5)+0.5*R(6))*MOLWT(1)*AREA0/1000.
C     YPRIME(2)=R(2)*EMAS(2)/EMASM*AREA0
C    1    -R(4)*MOLWT(2)*AREA0/1000.
C     YPRIME(3)=R(2)*EMAS(3)/EMASM*AREA0
C    1    +(R(4)-R(6))*MOLWT(3)*AREA0/1000.
C     YPRIME(4)=R(2)*EMAS(4)/EMASM*AREA0
C    1    +0.5*R(6)*MOLWT(4)*AREA0/1000.
C     YPRIME(5)=R(2)*EMAS(5)/EMASM*AREA0
C    1    +(2.*(LAMBDA(3)-1.)*R(3)+R(4)+2.*R(5))*MOLWT(5)*AREA0/1000.
C     YPRIME(6)=R(2)*EMAS(6)/EMASM*AREA0
C    1   +((2.-LAMBDA(3))*R(3)-R(5))*MOLWT(6)*AREA0/1000.
C     YPRIME(7)=-R(3)*MOLWT(7)*AREA0/1000.
C     YPRIME(8)=0.0
C     YPRIME(9)=-R(2)*AREA0+(YPRIME(1)-R(2)*EMAS(1)/EMASM*AREA0)
C     GO TO 712
C-----------------------------------------------------------------
 60   YPRIME(10)=Y(11)
      YPRIME(11)=((Y(9)*CPCOR(1)+1000.*(Y(2)*CPCOR(2)/MOLWT(2)
     1        +Y(3)*CPCOR(3)/MOLWT(3)+Y(4)*CPCOR(4)/MOLWT(4)
     1        +Y(5)*CPCOR(5)/MOLWT(5)+Y(6)*CPCOR(6)/MOLWT(6)
     2        +Y(7)*CPCOR(7)/MOLWT(7)+Y(8)*CPCOR(8)/MOLWT(8)))*Y(11)
     3        +DELH(2)*R(2)*AREA0-2.*3.1416*RAD0*HW*(TANN-Y(10)))
     4        /KEFF/AREA0
C     AX=(Y(9)*CPCOR(1)+1000.*(Y(2)*CPCOR(2)/MOLWT(2)+Y(3)*CPCOR(3)
C    1   /MOLWT(3)+Y(4)*CPCOR(4)/MOLWT(4)+Y(5)*CPCOR(5)/MOLWT(5)
C    2   +Y(6)*CPCOR(6)/MOLWT(6)+Y(7)*CPCOR(7)/MOLWT(7)+
C    3   Y(8)*CPCOR(8)/MOLWT(8)))*Y(11)
C     BX=+DELH(2)*R(2)*AREA0
C     CX=-2.*3.1416*RAD0*HW*(TANN-Y(10))
C     DX=KEFF*AREA0
      RETURN
C-----COMBUSTION ZONE -------------------------------------------
 70   CALL RATE(Y)
      YPRIME(1)=-(LAMBDA(3)*R(3)+R(4)+R(5)+0.5*R(6))*MOLWT(1)*AREA0
     1          /1000.
      YPRIME(2)=(-R(4)+RH2)*MOLWT(2)*AREA0/1000.
      YPRIME(3)=(R(4)-R(6)-RH2)*MOLWT(3)*AREA0/1000.
      YPRIME(4)=0.5*R(6)*MOLWT(4)*AREA0/1000.
      YPRIME(5)=(2.*(LAMBDA(3)-1.)*R(3)+R(4)+2.*R(5)-RCO)*MOLWT(5)
     1          *AREA0/1000.
```

```
      YPRIME(6)=((2.-LAMBDA(3))*R(3)-R(5)+RCO)*MOLWT(6)*AREAO/1000.
      XZ=ABS(Z-ZAIR)
      BET=FAIRIN/3.0554/WIDTH
      ABET=-(0.5*RH2+0.5*RCO+R(3))*MOLWT(7)*AREAO/1000.
      IF(XZ.GE.WIDTH)GO TO 75
      IF(XZ.LT.0.05385*WIDTH)GO TO 74
      BBET=0.233*BET*(-2.5*XZ/WIDTH+2.5)
      YPRIME(7)=-(0.5*RH2+0.5*RCO+R(3))*MOLWT(7)*AREAO/1000.
     1     +0.233*BET*(-2.5*XZ/WIDTH+2.5)
C     WRITE(6,73)Y(7),ABET,BBET,YPRIME(7)
C73   FORMAT(' OXY BAL',2X,G10.3,2X,G10.3,2X,G10.3,2X,G10.3)
      YPRIME(8)=0.767*BET*(-2.5*XZ/WIDTH+2.5)
      GO TO 76
 74   YPRIME(7)=-(0.5*RH2+0.5*RCO+R(3))*MOLWT(7)*AREAO/1000.
     1     +0.233*BET*(-200.4*XZ/WIDTH+13.1)
      BBET=0.233*BET*(-200.4*XZ/WIDTH+13.1)
C     WRITE(6,73)Y(7),ABET,BBET,YPRIME(7)
      YPRIME(8)=0.767*BET*(-200.4*XZ/WIDTH+13.1)
      GO TO 76
 75   YPRIME(7)=-(0.5*RH2+0.5*RCO+R(3))*MOLWT(7)*AREAO/1000.
      BBET=0.0
C     WRITE(6,73)Y(7),ABET,BBET,YPRIME(7)
      YPRIME(8)=0.0
 76   CONTINUE
C      YPRIME(7)=FAIRO
C      YPRIME(8)=FAIRN
C     OXY=Y(7)+FAIRO
C     OXYMOL=OXY*1000./MOLWT(7)
C     CHH2=0.5*Y(3)/MOLWT(3)*1000.
C     CHCH4=2.*Y(4)/MOLWT(4)*1000.
C     CHCO=0.5*Y(5)/MOLWT(5)*1000.
C     CHC =LAMBDA(3)*Y(1)/MOLWT(1)*1000.
C     WRITE(6,760)OXYMOL,CHH2,CHCH4,CHCO,CHC
C760  FORMAT('CH ',5(1X,G10.3))
C     IF(OXYMOL.LE.(0.5*Y(3)*1000./MOLWT(3)))GO TO 77
C     IF(OXYMOL.LE.((0.5*Y(3)/MOLWT(3)+2.*Y(4)/MOLWT(4))*1000.))
C    1   GO TO 78
C     IF(OXYMOL.LE.((0.5*Y(3)/MOLWT(3)+2.*Y(4)/MOLWT(4)
C    1   +0.5*Y(5)/MOLWT(5))*1000.))GO TO 79
C     IF(OXYMOL.LE.((0.5*Y(3)/MOLWT(3)+2.*Y(4)/MOLWT(4)
C    1   +0.5*Y(5)/MOLWT(5)+LAMBDA(3)*Y(1)/MOLWT(1))*1000.))GO TO 80
C77   YPRIME(7)=-Y(7)
C     YPRIME(8)=FAIRN
C     YPRIME(1)=0.0
C     YPRIME(2)=OXYMOL*2.
C     YPRIME(3)=-OXYMOL*2.
C     YPRIME(4)=0.0
C     YPRIME(5)=0.0
C     YPRIME(6)=0.0
C     WRITE(6,766)
C766  FORMAT(' COMB H2')
C     GO TO 81
C78   YPRIME(7)=-Y(7)
```

```
C      YPRIME(8)=FAIRN
C      YPRIME(1)=0.0
C      YPRIME(3)=-Y(3)
C      YPRIME(4)=-(OXYMOL-0.5*Y(3)*1000./MOLWT(3))*0.5*MOLWT(4)/1000.
C      YPRIME(5)=0.0
C      YPRIME(6)=-YPRIME(4)/MOLWT(4)*MOLWT(6)
C      YPRIME(2)=-(YPRIME(3)/MOLWT(3)+2.*YPRIME(4)/MOLWT(4))*MOLWT(2)
C      WRITE(6,767)
C767   FORMAT(' COMB H2 CH4')
C      GO TO 81
C79    YPRIME(7)=-Y(7)
C      YPRIME(8)=FAIRN
C      YPRIME(1)=0.0
C      YPRIME(3)=-Y(3)
C      YPRIME(4)=-Y(4)
C      YPRIME(5)=-(OXYMOL-(0.5*Y(3)/MOLWT(3)+2.*Y(4)/MOLWT(4))*1000.)
C     1      *2.*MOLWT(5)/1000.
C      YPRIME(6)=-(YPRIME(4)/MOLWT(4)+YPRIME(5)/MOLWT(5))*MOLWT(6)
C      YPRIME(2)=-(YPRIME(3)/MOLWT(3)+2.*YPRIME(4)/MOLWT(4))*MOLWT(2)
C      WRITE(6,768)
C768   FORMAT(' COMB H2 CH4 CO')
C      GO TO 81
C80    YPRIME(7)=-Y(7)
C      YPRIME(8)=FAIRN
C      YPRIME(1)=-(OXYMOL-(0.5*Y(3)/MOLWT(3)+2.*Y(4)/MOLWT(4)+
C     1       0.5*Y(5)/MOLWT(5))*1000.)*LAMBDA(3)*MOLWT(1)/1000.
C      YPRIME(3)=-Y(3)
C      YPRIME(4)=-Y(4)
C      YPRIME(5)=-Y(5)
C      YPRIME(2)=-(YPRIME(3)/MOLWT(3)+2.*YPRIME(4)/MOLWT(4))*MOLWT(2)
C      YPRIME(6)=-(YPRIME(4)/MOLWT(4)+YPRIME(5)/MOLWT(5))*MOLWT(6)
C      WRITE(6,769)
C769   FORMAT(' COMB H2 CH4 CO C')
 81    YPRIME(9)=YPRIME(1)
 712   YPRIME(10)=Y(11)
       YPRIME(11)=((Y(1)*CPCOR(1)+1000.*(Y(2)*CPCOR(2)/MOLWT(2)
      1+Y(3)*CPCOR(3)/MOLWT(3)+Y(4)*CPCOR(4)/MOLWT(4)+Y(5)*CPCOR(5)
      2/MOLWT(5)+Y(6)*CPCOR(6)/MOLWT(6)+Y(7)*CPCOR(7)/MOLWT(7)+
      3Y(8)*CPCOR(8)/MOLWT(8)))*Y(11)+YPRIME(8)/0.767*CPAIR*(TAIR-298.)+
      4(R(3)*DELH(3)+R(4)*DELH(4)+R(5)*DELH(5)+R(6)*DELH(6)/2.+RH2*DELH2
      5+RCO*DELCO)*AREA0-2.*3.1416*RAD0*HW*(TANN-Y(10)))/KEFF/AREA0
C      AX=(Y(1)*CPCOR(1)+1000.*(Y(2)*CPCOR(2)/MOLWT(2)
C     1         +Y(3)*CPCOR(3)/MOLWT(3)+Y(4)*CPCOR(4)/MOLWT(4)
C     2         +Y(5)*CPCOR(4)/MOLWT(4)+Y(5)*CPCOR(5)/MOLWT(5)
C     3         +Y(6)*CPCOR(6)/MOLWT(6)+Y(7)*CPCOR(7)/MOLWT(7)
C     4         +Y(8)*CPCOR(8)/MOLWT(8)))*Y(11)
C      BX=(R(3)*DELH(3)+R(4)*DELH(4)+R(5)*DELH(5)+R(6)*DELH(6)/2.
C     1    +RH2*DELH2+RCO*DELCO)*AREA0
C      CX=-2.*3.1416*RAD0*HW*(TANN-Y(10))
C      DX=KEFF*AREA0
       RETURN
C-----GASIFICATION ZONE ----------------------------------------
 90    CALL RATE(Y)
```

```
      YPRIME(1)=-(R(4)+R(5)+0.5*R(6))*MOLWT(1)*AREA0/1000.
      YPRIME(2)=-R(4)*MOLWT(2)*AREA0/1000.
      YPRIME(3)=(R(4)-R(6))*MOLWT(3)*AREA0/1000.
      YPRIME(4)=0.5*R(6)*MOLWT(4)*AREA0/1000.
      YPRIME(5)=(R(4)+2.*R(5))*MOLWT(5)*AREA0/1000.
      YPRIME(6)=-R(5)*MOLWT(6)*AREA0/1000.
      YPRIME(7)=0.0
      YPRIME(8)=0.0
      YPRIME(9)=YPRIME(1)
      YPRIME(10)=Y(11)
      YPRIME(11)=((Y(1)*CPCOR(1)+1000.*(Y(2)*CPCOR(2)/MOLWT(2)
     1           +Y(3)*CPCOR(3)/MOLWT(3)+Y(4)*CPCOR(4)/MOLWT(4)
     2           +Y(5)*CPCOR(5)/MOLWT(5)+Y(6)*CPCOR(6)/MOLWT(6)
     3           +Y(7)*CPCOR(7)/MOLWT(7)+Y(8)*CPCOR(8)/MOLWT(8)))*Y(11)
     4           +(R(4)*DELH(4)+R(5)*DELH(5)+R(6)*DELH(6)
     5           /2.)*AREA0-2.*3.1416*RAD0*HW*(TANN-Y(10)))/KEFF/AREA0
C     AX=(Y(1)*CPCOR(1)+1000.*(Y(2)*CPCOR(2)/MOLWT(2)
C    1         +Y(3)*CPCOR(3)/MOLWT(3)+Y(4)*CPCOR(4)/MOLWT(4)
C    2         +Y(5)*CPCOR(4)/MOLWT(4)+Y(5)*CPCOR(5)/MOLWT(5)
C    3         +Y(6)*CPCOR(6)/MOLWT(6)+Y(7)*CPCOR(7)/MOLWT(7)
C    4         +Y(8)*CPCOR(8)/MOLWT(8)))*Y(11)
C     BX=(R(4)*DELH(4)+R(5)*DELH(5)+R(6)*DELH(6)/2.)*AREA0
C     CX=-2.*3.1416*RAD0*HW*(TANN-Y(10))
C     DX=KEFF*AREA0
      RETURN
C-----ANNULUS - NO FURTHER REACTION ----------------------------
 95   YPRIME(1)=0.0
      YPRIME(2)=0.0
      YPRIME(3)=0.0
      YPRIME(4)=0.0
      YPRIME(5)=0.0
      YPRIME(6)=0.0
      YPRIME(7)=0.0
      YPRIME(8)=0.0
      YPRIME(9)=0.0
      YPRIME(10)=-(2.*3.1416*(RAD0*HW*(Y(10)-TCOR)+
     1           RAD2*HW0*(Y(10)-TAMB)))/(1000.*(Y(2)*CPANN(2)/MOLWT(2)
     2          +Y(3)*CPANN(3)/MOLWT(3)+Y(4)*CPANN(4)/MOLWT(4)
     3          +Y(5)*CPANN(5)/MOLWT(5)+Y(6)*CPANN(6)/MOLWT(6)
     4          +Y(7)*CPANN(7)/MOLWT(7)+Y(8)*CPANN(8)/MOLWT(8)))
      YPRIME(11)=0.0
      RETURN
      END
```

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C=======================================================================
      SUBROUTINE RATE(Y)
C=======================================================================
C     HERE THE GLOBAL REACTION RATES ARE COMPUTED FOR EACH
C     REACTION IN THE GASIFIER EXCEPT FOR DRYING AND THE
C     WATER-GAS SHIFT REACTION WHICH ARE ASSUMED TO BE AT
C     EQUILIBRIUM.
C-----------------------------------------------------------------------
      INTEGER        J(6),IFLAG(6)
      REAL           MWAVA,MWAVC,MOLWT,MWAIR,KGANN,KGCOR,KAIR,
     1               LAMBDA,KR(6),KP,PHI(6),ETA(6),KEFF,KS,Y(11),
     2               HD(7),KEQO(7)
      COMMON/PRINTX/KR
      COMMON/ANALYS/ANALA,ANALC,ANALH,ANALN,ANALO,PROXW,PROXC,
     1               PROXV,PROXA,PMOLO,PMOLC,PMOLH,EMAS(6),HCOMBW
      COMMON/DIMENS/RAD0,RAD1,RAD2,RAD3,AREA0
      COMMON/INPUT /TGUESS,RG,PRESS,TAMB,DP
      COMMON/LOCAL /IZ,ICOUNT,IFLAGA,JL,JJ,HW,HW0,R(6),RH2,RCO,
     1               DELH(7),DELH2,DELCO,DELTAZ,RECORE,DENSB,DENSP,
     2               FSTAR,TCORS,TCOR,TANN,GIBB(7),H2OSAT,
     3               KEFF,OPPOSE(9),GASFLO
      COMMON/PROPS /MOLWT(8),MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,
     1               VISANN,VISCOR,VISAIR,CPAVAN,CPANN(8),CPCOR(9),
     2               CPAIR,DIF(8),DEFF(8),LAMBDA(7),EMISS,COMPN(8),
     3               DENSGC,DENSGA,PP(8),PPEQ(8),CPAVCO,KS
      COMMON/WOOD  /FSO,DL,DH,DW,VOIDP,VOID,DENSBO,DENSPO
      DATA HD      /0.0,0.0,0.0,32457.,40300.,-21854.,-7860./
      DATA KEQO    /0.0,0.0,0.0,3.098E7,1.222E9,1.472E-6,0.0265/
C-----------------------------------------------------------------------
      SUM=Y(2)/MOLWT(2)+Y(3)/MOLWT(3)+Y(4)/MOLWT(4)+Y(5)/MOLWT(5)
     1   +Y(6)/MOLWT(6)+Y(7)/MOLWT(7)+Y(8)/MOLWT(8)
      DO 5 IJK=2,8
      PP(IJK)=Y(IJK)/MOLWT(IJK)/SUM*PRESS
      IF(PP(IJK).LT.0.0)PP(IJK)=0.0
 5    CONTINUE
      GO TO (10,20,20,20,40,50,60)ICOUNT
C-----DRYING ZONE - SATURATION AT LOCAL TEMPERATURE -------------
 10   DO 15 I5=1,6
      R(I5)=0.0
 15   CONTINUE
      RH2=0.0
      RCO=0.0
      RETURN
C-----PYROLYSIS ZONE --------------------------------------------
 20   CONV1=(FSTAR-Y(9))/FSTAR
      R(2)=2.667E8*DENSB*(1.-CONV1)*EXP(-(11072.+13588.*CONV1)
     1      /Y(10))
      IF(ICOUNT.EQ.4)GO TO 40
 32   RETURN
C-----COMBUSTION & GASIFICATION ZONES ---------------------------
 40   KR(3)=1.79E6*1000./MOLWT(1)*DENSP*EXP(-13588./Y(10))
      J(3)=7
 50   KR(4)=8.333E7*DENSP*(PP(2)/8.205E-5/Y(10))**0.7
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     1       /(PP(2)-PPEQ(2))*EXP(-217100./8.314/Y(10))
      J(4)=2
      KR(5)=8.333E7*DENSP*(PP(6)/8.205E-5/Y(10))**0.7
     1       /(PP(6)-PPEQ(6))*EXP(-217100./8.314/Y(10))
      J(5)=6
      CONV2=(FSTAR-Y(9))/FSTAR
      KR(6)=1.34E7*(1.-CONV2)*DENSP*
     1       EXP(-(13598.-3422.*CONV2+20101.*CONV2**2)/Y(10))
     2       *PP(3)/(PP(3)-PPEQ(3))
      J(6)=3
      IF(ICOUNT.EQ.6)GO TO 54
      M1=3
      GO TO 70
 54   M1=4
      GO TO 70
C-----ANNULUS - NO FURTHER REACTION ----------------------------
 60   RETURN
C---------------------------------------------------------------
 70   DO 110 I=M1,6
      IF((PP(J(I))-PPEQ(J(I))).LE.0.0)GO TO 111
      KP=2.06/(RECORE**0.575)*(DENSGC*DIF(J(I))/VISCOR)**0.666666
     1       *737.3/MWAVC*(Y(2)+Y(3)+Y(4)+Y(5)+Y(6)+Y(7)+Y(8))
     2       /(3.1416*(RADO**2))*1.35625/VOID/(PRESS-PP(J(I)))
     3       *(1.-VOID)
      DENSG1=PRESS*MWAVC/8.205E-5/Y(10)/1000.
C-----SHRINKING CORE MODEL -------------------------------------
C     ASTAR=FSO*ANALA/(1.+PROXW)/FSTAR
C     RF=(Y(9)-FSTAR*ASTAR)/(FSTAR*(1.-ASTAR))
C     PHI(I)=(DL**2./DIF(J(I))*KR(I)*8.205E-5*Y(10)/(1.-VOID))**0.5
C     IF(PHI(I).GT.4)GO TO 75
C     SINH=(EXP(PHI(I))-EXP(-PHI(I)))/2.
C     COSH=(EXP(PHI(I))+EXP(-PHI(I)))/2.
C     ETA(I)=1./PHI(I)*SINH/COSH
C     GO TO 80
C75   ETA(I)=1./PHI(I)
C80   IF((KP.EQ.0.).OR.(KR(I).EQ.0.))GO TO 111
C     IF(DEFF(J(I)).EQ.0.)GO TO 111
C     R(I)=(1.-VOID)*(PP(J(I))-PPEQ(J(I)))/
C    1 (DL/KP + DL**2.*(1.-RF)*8.205E-5*Y(10)/DEFF(J(I))
C    2        + 1./(RF*ETA(I)*KR(I)))
C-----ASH SEGREGATION MODEL ------------------------------------
      RF=Y(9)/FSTAR
      IF((KP.EQ.0.).OR.(KR(I).EQ.0.))GO TO 111
      R(I)=(1.-VOID)*(PP(J(I))-PPEQ(J(I)))/
     1  (RF*DL/KP/3. + 1./KR(I))
C---------------------------------------------------------------
 104  IF((Y(1).LE.0.).OR.(Y(7).LE.0.))R(3)=0.0
      IF((Y(1).LE.0.).OR.(Y(2).LE.0.))R(4)=0.0
      IF((Y(1).LE.0.).OR.(Y(6).LE.0.))R(5)=0.0
      IF((Y(1).LE.0.).OR.(Y(3).LE.0.))R(6)=0.0
      IF(R(I).LE.0.)GO TO 111
      GO TO 110
 111  R(I)=0.0
```

```
110   CONTINUE
      RH2=12.E10*EXP(-8052.3/Y(10))*(PRESS/82.05/Y(10))**1.8
     2  *(PP(7)**0.3)*(PP(2)**0.4)*PP(3)*1000000./(PRESS**1.7)
      RCO=12.E10*EXP(-8052.3/Y(10))*(PRESS/82.05/Y(10))**1.8
     1  *(PP(7)**0.3)*(PP(2)**0.4)*PP(5)*1000000./(PRESS**1.7)
      IF((Y(3).LE.0.).OR.(Y(7).LE.0.))RH2=0.0
      IF((Y(5).LE.0.).OR.(Y(7).LE.0.))RCO=0.0
      RETURN
      END
```

```
C=======================================================================
      SUBROUTINE PRPTYS(Y)
C=======================================================================
C     THIS IS THE PHYSICAL PROPERTY PACKAGE, INCLUDING THERMAL
C     CONDUCTIVITY, VISCOSITY, HEAT CAPACITY, DIFFUSIVITY,
C     DENSITY AND EMISSIVITY.
C-----------------------------------------------------------------------
      REAL           MOLWT,MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,
     1               LAMBDA,IDD(50),ID,MOLWAV,NUMERK,NUMERV,
     2               KK(9),CCP(9),XG(8),COL(8),EKT(50),
     3               EK(8),VVISC(9),D(8,8),DIFINV(8),Y(11),KEFF,
     4               OPPO(8),XOPPO(8),XMOL(8),KS
      COMMON/ANALYS/ANALA,ANALC,ANALH,ANALN,ANALO,PROXW,PROXC,
     1               PROXV,PROXA,PMOLO,PMOLC,PMOLH,EMAS(6),HCOMBW
      COMMON/GAS    /FAIRIN,EH2O,EO2,EN2,TAIR,PAIR,FAIR,
     1               ZL,ZAIR,WIDTH
      COMMON/INPUT  /TGUESS,RG,PRESS,TAMB,DP
      COMMON/LOCAL  /IZ,ICOUNT,IFLAGA,JL,JJ,HW,HWO,R(6),RH2,RCO,
     1               DELH(7),DELH2,DELCO,DELTAZ,RECORE,DENSB,DENSP,
     2               FSTAR,TCORS,TCOR,TANN,GIBB(7),H2OSAT,
     3               KEFF,OPPOSE(9),GASFLO
      COMMON/PROPS  /MOLWT(8),MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,
     1               VISANN,VISCOR,VISAIR,CPAVAN,CPANN(8),CPCOR(9),
     2               CPAIR,DIF(8),DEFF(8),LAMBDA(7),EMISS,COMPN(8),
     3               DENSGC,DENSGA,PP(8),PPEQ(8),CPAVCO,KS
      COMMON/WOOD   /FSO,DL,DH,DW,VOIDP,VOID,DENSBO,DENSPO
      DATA EK/0.0,363.,33.3,136.5,110.3,190.,113.2,91.5/
      DATA EKT/.3,.4,.5,.6,.7,.8,.9,1.,1.1,1.2,1.3,1.4,1.5,1.6,1.7,
     1    1.8,1.9,2.,2.2,2.4,2.6,2.8,3.0,3.2,3.4,3.6,3.8,4.,4.2,4.4,
     2    4.6,4.8, 5.,6.,7.,8.,9.,10.,20.,30.,40.,50.,60.,70.,80.,90.
     3    ,100.,200., 300.,400./
      DATA IDD/1.331,1.159,1.033,.9383,.8644,.8058,.7585,.7197,.6873,
     1  .66,.6367,.6166,.5991,.5837,.5701,.558,.5471,.5373,.5203,.5061,
     2 .494,.4836,.4745,.4664,.4593,.4529,.4471,.4418,.437,.4326,.4284,
     3  .4246,.4211,.4062,.3948,.3856,.3778,.3712,.332,.3116,.298,.2878
     4  ,.2798,.2732,.2676,.2628,.2585,.2322,.218,.2085/
      DATA COL/0.,2.655,2.968,3.882,3.590,3.996,3.433,3.681/
C-----PACKED BED AND PARTICLE DENSITIES ------------------------
      DENSB=DENSBO*Y(9)/FSO
      DENSP=DENSPO*Y(9)/FSO
      IF(ICOUNT.GT.2)VOIDPL=VOIDP+(FSTAR-Y(9))/FSTAR*(1.-VOIDP)
C-----------------------------------------------------------------------
      IF(IFLAGA.NE.0)GO TO 51
C
C-----ELEMENTAL COMPOSITION OF WOOD (MOLAR BASIS) ---------------
      SUM1=ANALC/12.01115 + ANALH/1.0079 + ANALN/14.0067 +
     1     ANALO/15.9994 + ANALA/64.65
      AMOLC=ANALC/12.01115/SUM1
      AMOLH=ANALH/1.0079  /SUM1
      AMOLN=ANALN/14.0067 /SUM1
      AMOLO=ANALO/15.9994 /SUM1
      AMOLA=ANALA/64.65   /SUM1
C
```

```
C-----ELEMENTAL COMPOSITION OF PYROLYSIS PRODUCTS (MOLAR BASIS) --
      SUM2=(ANALC-PROXC)/12.01115 + ANALO/15.9994 + ANALH/1.0079
      PMOLC=(ANALC-PROXC)/12.01115/SUM2
      PMOLH=ANALH/1.0079 /SUM2
      PMOLO=ANALO/15.9994/SUM2
C
C-----EMISSIVITY ----------------------------------------------------
      EMISS=0.95
C
C-----STOICHIOMETRIC COEFFICIENTS -----------------------------------
      DO 10 J=1,7
      LAMBDA(J)=1.0
   10 CONTINUE
C     COMBUSTION STOICHIOMETRY
   51 XI=218.*EXP(-7250./Y(10))
      LAMBDA(3)=2.*(XI+1.)/(2.+XI)
C-------------------------------------------------------------------
      DO 30 I=1,8
      COMPN(I)=Y(I)*1000./MOLWT(I)
      OPPO(I)=OPPOSE(I)*1000./MOLWT(I)
   30 CONTINUE
      FLOWNT=COMPN(2)+COMPN(3)+COMPN(4)+COMPN(5)+COMPN(6)
     1       +COMPN(7)+COMPN(8)
      SUMOPP=OPPO(2)+OPPO(3)+OPPO(4)+OPPO(5)+OPPO(6)+OPPO(7)+OPPO(8)
      DO 50 IY=2,8
      XG(IY)=COMPN(IY)/FLOWNT
      PP(IY)=XG(IY)*PRESS
      XOPPO(IY)=OPPO(IY)/SUMOPP
   50 CONTINUE
C
   60 IF(Z.GE.ZL)GO TO 70
C     IN PACKED BED
      T1=TANN
      T2=Y(10)
      GO TO 80
C     IN ANNULUS
   70 T1=Y(10)
      T2=TCOR
   80 CONTINUE
      DO 190 II=1,2
C     COMPUTE ANNULAR CONDITIONS
      IF(II.EQ.1)T=T1
C     COMPUTE PACKED BED CONDITIONS
      IF(II.EQ.2)T=T2
      IF((II.EQ.1.AND.ICOUNT.NE.7).OR.(II.EQ.2.AND.ICOUNT.EQ.7))
     1     GO TO 85
      DO 82 KJ=2,8
      XMOL(KJ)=XG(KJ)
   82 CONTINUE
      GO TO 100
   85 DO 86 KL=2,8
      XMOL(KL)=XOPPO(KL)
   86 CONTINUE
```

```
C
C-----HEAT CAPACITY (J/MOL K) EXCEPT CCP(9)=J/KG K ---------------
  100 CCP(1)=( 4.03+ 1.14E-3*T -2.04E5/T**2)  * 4.184
      CCP(2)=( 7.30+ 2.46E-3*T) * 4.184
      CCP(3)=( 6.52+ 0.78E-3*T + 0.12E5/T**2) * 4.184
      CCP(4)=(3.381+18.044E-3*T-4.300E-6*T**2)* 4.184
      CCP(5)=( 6.79+ 0.98E-3*T -0.11E5/T**2)  * 4.184
      CCP(6)=(10.57+ 2.10E-3*T -2.06E5/T**2)  * 4.184
      CCP(7)=( 7.16+ 1.00E-3*T -0.40E5/T**2)  * 4.184
      CCP(8)=( 6.83+ 0.90E-3*T -0.12E5/T**2)  * 4.184
C     CCP(9)=0.57*4184.
      CCP(9)=(0.266 + 0.00116*(T-273.2))*4.184*1000.
C
C-----THERMAL CONDUCTIVITY  (J/S M K) ----------------------------
      KK(1)=(0.020 + 1.25E-5*T)*100.
      KK(2)=-3.15333E-2 + 0.145714E-3*T -0.266667E-7*T**2
      KK(3)=7.777198E-2 + 0.362363E-3*T -0.120879E-7*T**2
      KK(4)=0.00994014E-2 + 0.0772505E-3*T +0.818226E-7*T**2
      KK(5)=1.10418E-2  + 0.059247E-3*T -0.057967E-7*T**2
      KK(6)=-1.95682E-2 + 0.119447E-3*T -0.317582E-7*T**2
      KK(7)=0.618402E-2 + 0.0763505E-3*T -0.108331E-7*T**2
      KK(8)=0.939180E-2 + 0.0642581E-3*T -0.105185E-7*T**2
      KK(9)=(DENSPO/1000.*(1.39 + 0.028*PROXW*100.)+0.165)*1.7307/12.
      IF((ICOUNT.EQ.4).OR.(ICOUNT.EQ.5).OR.(ICOUNT.EQ.6))GO TO 101
      KS=KK(9)
      GO TO 102
  101 KS=KK(1)
C
C-----VISCOSITY  (N S / M2) --------------------------------------
  102 VVISC(1)=0.
      VVISC(2)=(80.4 + 0.407*(T-273.2))*1.0E-7
      VVISC(3)=5.579E-6 +0.0151E-6*T
      VVISC(4)=7.384E-6 +0.0204E-6*T
      VVISC(5)=14.380E-6 + 0.026E-6*T
      VVISC(6)=10.389E-6 + 0.029E-6*T
      VVISC(7)=15.651E-6 + 0.0327E-6*T
      VVISC(8)=14.389E-6 + 0.0257E-6*T
      VVISC(9)=0.0
C
C-----DIFFUSION COEFFICIENTS (M2/S) ------------------------------
      D(1,1)=0.
      D(1,2)=0.
      D(2,1)=0.
      DO 120 J9=2,8
      DO 110 I9=2,8
      DUM1=T/(EK(I9)*EK(J9))**0.5
      CALL INTERP(50,EKT,IDD,ID,DUM1)
      COLD=(COL(I9)+COL(J9))/2.
      DUM2=(10.85-2.50*((1./MOLWT(I9)+1./MOLWT(J9))**0.5))*1.0E-4
      D(I9,J9)=DUM2*T**1.5*((1./MOLWT(I9)+1./MOLWT(J9))**0.5)
     1       /PRESS/COLD**2./ID*1.0E-4
  110 CONTINUE
  120 CONTINUE
```

```
C
C-----GAS MIXTURE PROPERTIES ------------------------------------
      MOLWAV=0.
      NUMERK=0.
      DENOMK=0.
      NUMERV=0.
      DENOMV=0.
      DIFINV(1)=0.
      DO 140 I8=2,8
      MOLWAV=MOLWAV+ XMOL(I8)*MOLWT(I8)
      NUMERK=NUMERK+ XMOL(I8)*KK(I8)*MOLWT(I8)**0.333333
      DENOMK=DENOMK+ XMOL(I8)*MOLWT(I8)**0.333333
      NUMERV=NUMERV+ XMOL(I8)*VVISC(I8)*MOLWT(I8)**0.5
      DENOMV=DENOMV+ XMOL(I8)*MOLWT(I8)**0.5
      DIFINV(I8)=0.
      IF((ICOUNT.EQ.1).OR.(ICOUNT.EQ.2))GO TO 140
      DO 130 J8=2,8
      DIFINV(I8)=DIFINV(I8) + XMOL(J8)/D(I8,J8)
 130  CONTINUE
      DIF(I8)=(1.-XMOL(I8))/(DIFINV(I8)-XMOL(I8)/D(I8,I8))
C-----EFFECTIVE DIFFUSIVITY OF GAS IN WOOD CHAR PARTICLE --------
      IF(VOIDPL.LE.0.75)DEFF(I8)=0.01*DIF(I8)
      IF((VOIDPL.GT.0.75).AND.(VOIDPL.LT.0.84))DEFF(I8)=DIF(I8)*
     1       (7.69*VOIDPL-5.62)
      IF((VOIDPL.GE.0.84).AND.(VOIDPL.LT.1.00))DEFF(I8)=DIF(I8)*VOIDPL
 140  CONTINUE
      IF(II.EQ.2)GO TO 160
C
C-----ANNULAR CONDITIONS ----------------------------------------
      KGANN=NUMERK/DENOMK
      VISANN=NUMERV/DENOMV
      MWAVA=MOLWAV
      CPAVAN=0.0
      DO 150 KJJ=2,8
      CPANN(KJJ)=CCP(KJJ)
      CPAVAN=CPAVAN+CPANN(KJJ)*XMOL(KJJ)
 150  CONTINUE
      CPAVAN=CPAVAN*1000./MWAVA
      DENSGA=MWAVA*PRESS/(T1*8.205E-5*1000.)
      GO TO 190
C-----PACKED BED CONDITIONS -------------------------------------
 160  KGCOR=NUMERK/DENOMK
      VISCOR=NUMERV/DENOMV
      MWAVC=MOLWAV
      CPAVCO=0.0
      DO 170 JK=2,8
      CPCOR(JK)=CCP(JK)
      CPAVCO=CPAVCO+CPCOR(JK)*XMOL(JK)
 170  CONTINUE
      CPCOR(9)=CCP(9)
      CPCOR(1)=CCP(1)*1000./12.
      CPAVCO=CPAVCO*1000./MWAVC
      DENSGC=MWAVC*PRESS/(T2*8.205E-5*1000.)
```

```
 190  CONTINUE
      IF(IFLAGA.EQ.1)GO TO 210
C
C-----PROPERTIES OF AIR AT AMBIENT TEMPERATURE ------------------
C     YET TO BE CORRECTED TO ACCOUNT FOR HUMIDITY
      T=TAMB
      CCP(7)=( 7.16+ 1.00E-3*T -0.40E5/T**2)  * 4.184
      CCP(8)=( 6.83+ 0.90E-3*T -0.12E5/T**2)  * 4.184
      KK(7)=0.618402E-2 + 0.0763505E-3*T -0.108331E-7*T**2
      KK(8)=0.939180E-2 + 0.0642581E-3*T -0.105185E-7*T**2
      VVISC(7)=15.651E-6 + 0.0327E-6*T
      VVISC(8)=14.389E-6 + 0.0257E-6*T
      IFLAGA=1
      MWAIR=0.21*MOLWT(7)+0.79*MOLWT(8)
      CPAIR=(0.21*CCP(7) + 0.79*CCP(8))*1000./MWAIR
      KAIR =0.21*KK(7)*MOLWT(7)**0.333333 + 0.79*KK(8)*MOLWT(8)
     1       **0.333333/(0.21*MOLWT(7)**0.333333+0.79*MOLWT(8)
     2       **0.333333)
      VISAIR=(0.21*VVISC(7)*MOLWT(7)**0.5 + 0.79*VVISC(8)*MOLWT(8)
     1       **0.5)/(0.21*MOLWT(7)**0.5 + 0.79*MOLWT(8)**0.5)
C-----------------------------------------------------------------
 210  RETURN
      END
```

```
C=======================================================================
      SUBROUTINE HTCOF(Y)
C=======================================================================
C     HEAT TRANSFER COEFFICIENTS ACROSS THE INNER AND OUTER WALLS
C     OF THE GASIFIER AND THE AXIAL THERMAL CONDUCTIVITY ARE
C     COMPUTED HERE.
C-----------------------------------------------------------------------
      REAL           MOLWT,MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,KW,
     1               LAMBDA,KEFF,KEO,YCOR(8),YANN(8),KS,Y(11)
      COMMON/GAS    /FAIRIN,EH2O,EO2,EN2,TAIR,PAIR,FAIR,
     1               ZL,ZAIR,WIDTH
      COMMON/DIMENS/RAD0,RAD1,RAD2,RAD3,AREA0
      COMMON/INPUT /TGUESS,RG,PRESS,TAMB,DP
      COMMON/LOCAL /IZ,ICOUNT,IFLAGA,JL,JJ,HW,HWO,R(6),RH2,RCO,
     1               DELH(7),DELH2,DELCO,DELTAZ,RECORE,DENSB,DENSP,
     2               FSTAR,TCORS,TCOR,TANN,GIBB(7),H2OSAT,KEFF,
     3               OPPOSE(9),GASFLO
      COMMON/PROPS /MOLWT(8),MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,
     1               VISANN,VISCOR,VISAIR,CPAVAN,CPANN(8),CPCOR(9),
     2               CPAIR,DIF(8),DEFF(8),LAMBDA(7),EMISS,COMPN(8),
     3               DENSGC,DENSGA,PP(8),PPEQ(8),CPAVCO,KS
      COMMON/WOOD  /FSO,DL,DH,DW,VOIDP,VOID,DENSBO,DENSPO
C-----------------------------------------------------------------------
      IF(ICOUNT.EQ.7)GO TO 10
C-----LOCALE IS CORE -------------------------------------------------
      DO 5 I=2,8
      YCOR(I)=Y(I)
      YANN(I)=OPPOSE(I)
   5  CONTINUE
      GO TO 20
C-----LOCALE IS ANNULUS ----------------------------------------------
  10  DO 12 J=2,8
      YCOR(J)=OPPOSE(J)
      YANN(J)=Y(J)
  12  CONTINUE
  20  IF(JJ.GT.1)GO TO 25
      VELANN=2.6*8.205E-5*TANN/PRESS/(3.1416*(RAD2**2-RAD1**2))
      GO TO 30
  25  VELANN=GASFLO*8.205E-5*TANN/PRESS/(3.1416*(RAD2**2-RAD1**2))
  30  DEQ=2.*(RAD2-RAD1)
C-----NATURAL CONVECTION ON OUTSIDE WALL -----------------------------
      GR=(MWAIR/8.205E-5/1000.*PRESS)**2.*((1./TANN+1./TAMB)/2.)**2.
     1    *0.00367*0.980665*(2.*RAD3)**3.*(TANN-TAMB)/VISAIR**2.
      PRAIR=CPAIR*VISAIR/KAIR
C     IF((PRAIR.LT.1.).OR.(PRAIR.GT.40.))
C    1    WRITE(6,100)CPAIR,VISAIR,KAIR,TAMB
      IF(GR.LT.1.E-9)GO TO 40
      HNC=0.683*(GR*PRAIR)**0.25*(PRAIR/(0.861+PRAIR))**0.25
     1     *KAIR/(2.*RAD3)
      GO TO 50
 40   HNC=0.138*GR**0.36*(PRAIR**0.175-0.55)*KAIR/(2.*RAD3)
C-----THERMAL CONDUCTIVITY OF WALL -----------------------------------
 50   KW=50.
```

```
C-----ANNULAR COEFFICIENTS ----------------------------------------
      REANN =DEQ*VELANN*DENSGA/VISANN
      PRANN=CPAVAN*VISANN/KGANN
      GRANNI=(MWAVA/8.205E-5/1000.*PRESS)**2.*((1./TCOR+1./TANN)/2.)
     1  **2.*0.00367*0.980665*((RAD2-RAD1)/2.)**3.*ABS(TCOR-TANN)
     2 /(VISANN**2.)
      GRANNO=(MWAVA/8.205E-5/1000.*PRESS)**2.*((1./TANN+1./TAMB)/2.)
     1  **2.*0.00367*0.980665*((RAD2-RAD1)/2.)**3.*ABS(TANN-TAMB)
     2 /(VISANN**2.)
      HFCI=1.02*KGANN/DEQ*(REANN**0.45)*(PRANN**0.5)*((DEQ/ZL)**0.4)
     1     *((RAD2/RAD1)**0.8)*(GRANNI**0.05)
      HFCO=1.02*KGANN/DEQ*(REANN**0.45)*(PRANN**0.5)*((DEQ/ZL)**0.4)
     1     *((RAD2/RAD1)**0.8)*(GRANNO**0.05)
C     HFCI=0.023*KGANN/DEQ*(DEQ*VELANN*DENSGA/VISANN)**0.8*
C    1       (CPAVAN*VISANN/KGANN)**0.4*(RAD2/RAD1)**0.45
C     HFCO=0.023/(DEQ*VELANN*DENSGA/VISANN)**0.2/
C    1       (CPAVAN*VISANN/KGANN)**0.666666*VELANN*DENSGA*CPAVAN
C-----PACKED BED COEFFICIENT -------------------------------------
      RECORE=DP*(YCOR(2)+YCOR(3)+YCOR(4)+YCOR(5)+YCOR(6)+YCOR(7)+
     1       YCOR(8))/AREAO/VISCOR
      IF(ICOUNT.EQ.5)GO TO 60
      HPB=0.813*KGCOR/(2.*RADO)*EXP(-6.*DP/(2.*RADO))*RECORE**0.9
      GO TO 70
 60   HPB=3.6*KGCOR/DP*(RECORE/VOID)**0.365
C-----------------------------------------------------------------
 70   ALM01=(RAD1-RADO)/ALOG(RAD1/RADO)*2.*3.1416
      ALM23=(RAD3-RAD2)/ALOG(RAD3/RAD2)*2.*3.1416
      AREAI=2.*3.1416*RADO
      AREA1=2.*3.1416*RAD1
      AREA2=2.*3.1416*RAD2
      AREA3=2.*3.1416*RAD3
C-----OVERALL HEAT TRANSFER COEFFICIENTS --------------------------
      HW=1./(AREA1/AREAI/HPB+(RAD1-RADO)*AREA1/ALM01/KW+1./HFCI)
      HWO=1./(AREA3/AREA2/HFCO+(RAD3-RAD2)*AREA3/ALM23/KW+1./HNC)
C-----AXIAL CONDUCTION --------------------------------------------
      HRV=0.1952*(TCOR/100.)**3/(1.+VOID/2./(1.-VOID)*(1.-EMISS)
     1       /EMISS)
      HRS=0.1952*EMISS/(2.-EMISS)*(TCOR/100.)**3
      KEO=KGCOR*(1.-VOID)/(KGCOR/KS+1./(29.412+DP*HRS/0.86042/KGCOR))
     1       +VOID*DP*HRV/0.86042/KGCOR
      PRCOR=CPAVCO*VISCOR/KGCOR
      IF(ICOUNT.GT.2)SCCOR=VISCOR/DENSGC/DIF(8)
      PEHCOR=RECORE*PRCOR
      PEMCOR=RECORE*SCCOR
      KEFF=KGCOR*(KEO/KGCOR+0.14*PRCOR*RECORE)
C-----------------------------------------------------------------
 100  FORMAT(' HNC CORRELATION NOT APPROPRIATE IN HTCOF',/,
     1       ' CPAIR,VISAIR,KAIR,TAMB',2X,G10.2,2X,G10.2,2X,G10.2
     2       ,2X,G10.2)
      RETURN
      END
```

```
C=======================================================================
      SUBROUTINE DELTAH(Y)
C=======================================================================
C     THE ENTHALPY FOR EACH REACTION IS COMPUTED AS A FUNCTION
C     OF THE REACTION TEMPERATURE.
C-----------------------------------------------------------------------
      REAL           LAMBDA,MOLWT,MWAVA,MWAVC,MWAIR,KGANN,KGCOR,
     1               KAIR,Y(11),KEFF,KS
      COMMON/ANALYS/ANALA,ANALC,ANALH,ANALN,ANALO,PROXW,PROXC,
     1               PROXV,PROXA,PMOLO,PMOLC,PMOLH,EMAS(6),HCOMBW
      COMMON/LOCAL /IZ,ICOUNT,IFLAGA,JL,JJ,HW,HWO,R(6),RH2,RCO,
     1               DELH(7),DELH2,DELCO,DELTAZ,RECORE,DENSB,DENSP,
     2               FSTAR,TCORS,TCOR,TANN,GIBB(7),H2OSAT,
     3               KEFF,OPPOSE(9),GASFLO
      COMMON/PROPS /MOLWT(8),MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,
     1               VISANN,VISCOR,VISAIR,CPAVAN,CPANN(8),CPCOR(9),
     2               CPAIR,DIF(8),DEFF(8),LAMBDA(7),EMISS,COMPN(8),
     3               DENSGC,DENSGA,PP(8),PPEQ(8),CPAVCO,KS
C-----------------------------------------------------------------------
      T=Y(10)
      DELH(1)=(-10.70*T+1.23E-3*T**2+13598.)*4.184
      DELH(3)=(0.40*T+0.62E-3*T**2+3.50E5/T-136618.75+
     1       LAMBDA(3)*(-1.020*T-0.64E-3*T**2-3.88E5/T+42881.80))
     2       *4.184
      DELH(4)=(1.98*T-0.92E-3*T**2-2.05E5/T+31561.58)*4.184
      DELH(5)=(-1.02*T-0.64E-3*T**2-3.88E5/T+42881.81)*4.184
      DELH(6)=(-13.69*T+7.67E-3*T**2-1.80E5/T-1.43E-6*T**3
     1       -13848.55)*4.184
      DELH2 =(-2.8*T+0.59E-3*T**2-0.08E5/T-56989.)*4.184
      DELCO =(0.2*T+0.31E-3*T**2+1.75E5/T-68309.)*4.184
C-----HEAT OF PYROLYSIS ---------------------------------------
      IF(ICOUNT.NE.2.AND.ICOUNT.NE.3.AND.ICOUNT.NE.4)GO TO 10
      CALL PYROL(Y)
      HCOMBW=-232596.*(146.58*ANALC+568.78*ANALH+.2945-
     1       6.58*ANALA-51.53*(ANALO+ANALN))
      HCOMBP=(PROXC+PROXV*EMAS(1))*(-3.2792E7)
     1        +PROXV*EMAS(2)*(-2.4451E6)+PROXV*EMAS(3)*(-1.4292E8)
     2        +PROXV*EMAS(4)*(-5.5647E7)+PROXV*EMAS(5)*(-1.0107E7)
      HCPDT1=348.67*(PROXC+PROXV*EMAS(1))*
     1        (4.03*T+0.57E-3*T**2+2.04E5/T-1936.12)
     1       +232.44*EMAS(2)*(7.30*T+1.23E-3*T**2-2284.63)
     2       +2092.*EMAS(3)*(6.52*T+0.39E-3*T**2-0.12E5/T-1937.33)
     3       +261.5*EMAS(4)*(3.381*T+9.022E-3*T**2-1.43E-6*T**3-
     4        1770.88)
      HCPDT2= 149.43*EMAS(5)*(6.79*T+0.49E-3*T**2+0.11E5/T-2103.85)
     6       +95.09*EMAS(6)*(10.57*T+1.05E-3*T**2+2.06E5/T-3934.38)
      HCPDT3=-(-212.04*T+2.427*T**2-152351.)
      HCPDT=HCPDT1+HCPDT2+HCPDT3
      DELH(2)=HCOMBW-HCOMBP+HCPDT
C-----------------------------------------------------------------------
  10  RETURN
      END
```

```
C=====================================================================
      SUBROUTINE PYROL(Y)
C=====================================================================
C     THE PYROLYSIS PRODUCT DISTRIBUTION IS COMPUTED AS A
C     FUNCTION OF TEMPERATURE.
C---------------------------------------------------------------------
      REAL           MOLWT,MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,
     1               LAMBDA,Y(11),KEFF,KS
      DIMENSION      ROO(8),RHH(8),TEMP(8),W(6),EMOL(6)
      COMMON/ANALYS/ANALA,ANALC,ANALH,ANALN,ANALO,PROXW,PROXC,
     1               PROXV,PROXA,PMOLO,PMOLC,PMOLH,EMAS(6),HCOMBW
      COMMON/LOCAL /IZ,ICOUNT,IFLAGA,JL,JJ,HW,HWO,R(6),RH2,RCO,
     1               DELH(7),DELH2,DELCO,DELTAZ,RECORE,DENSB,DENSP,
     2               FSTAR,TCORS,TCOR,TANN,GIBB(7),H2OSAT,
     3               KEFF,OPPOSE(9),GASFLO
      COMMON/PROPS /MOLWT(8),MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,
     1               VISANN,VISCOR,VISAIR,CPAVAN,CPANN(8),CPCOR(9),
     2               CPAIR,DIF(8),DEFF(8),LAMBDA(7),EMISS,COMPN(8),
     3               DENSGC,DENSGA,PP(8),PPEQ(8),CPAVCO,KS
C     RH=CH4/CO2     RC=C/CO2
C     MAA DISTRIBUTION
C     DATA ROO/0.59,0.59,0.48,0.41,1.16,2.17,2.52,2.65/
C     DATA RHH/0.   ,0.   ,0.13,0.23,0.39,0.63,0.71,0.75/
C     SIMMONS DISTRIBUTION
C     DATA ROO/0.43,0.75,1.16,1.96,2.61,4.45,12.5,50./
C     DATA RHH/0.   ,0.   ,0.24,0.61,0.67,0.91,2.   ,7. /
C-----AVERAGE DISTRIBUTION ------------------------------------
      DATA RHH/0.70,0.70,0.85,1.00,1.15,1.30,1.30,1.30/
      DATA TEMP/300.,400.,500.,600.,700.,800.,900.,1000./
C---------------------------------------------------------------------
      NPTSP=8
      TBAR=Y(10)-273.2
      RC=0.0
      CALL INTERP(NPTSP,TEMP,RHH,RH,TBAR)
      A=(0.85*RH-0.15)/0.15
      B=((RC+RH+1.)*PMOLO-2.*PMOLC)/PMOLC
      C=(PMOLO-PMOLC)/PMOLC
      D=(PMOLH*(2.+B)-2.*PMOLO*(A+B+2.*RH))/(2.*PMOLO*(C-1.)-
     1   PMOLH*(1.+C))
      EMOL(6)=1./(1.+RC+RH+A+B+C*D)
      EMOL(5)=EMOL(6)*D
      EMOL(4)=EMOL(6)*RH
      EMOL(3)=EMOL(6)*A-EMOL(5)
      EMOL(1)=EMOL(6)*RC
      EMOL(2)=1.-(EMOL(1)+EMOL(3)+EMOL(4)+EMOL(5)+EMOL(6))
C-----CONVERT TO MASS FRACTIONS -------------------------------
      SUM=0.
      DO 10 I=1,6
      W(I)=EMOL(I)*MOLWT(I)
      SUM=SUM+W(I)
```

```
10    CONTINUE
      DO 20 I=1,6
      EMAS(I)=W(I)/SUM
20    CONTINUE
      RETURN
      END
```

```
C=======================================================================
      SUBROUTINE GEOMTY(Z)
C=======================================================================
C     THE DIMENSIONS WHICH ARE CURRENTLY BEING USED ARE THOSE
C     OF THE IMBERT DOWN-DRAFT GASIFIER BEING OPERATED BY
C     SASKATCHEWAN POWER CORP. IN REGINA.
C-----------------------------------------------------------------------
      REAL            KEFF
      DIMENSION       ZZ(13),DIA1(13)
      COMMON/DIMENS/RAD0,RAD1,RAD2,RAD3,AREA0
      COMMON/GAS    /FAIRIN,EH2O,EO2,EN2,TAIR,PAIR,FAIR,
     1               ZL,ZAIR,WIDTH
      COMMON/LOCAL /IZ,ICOUNT,IFLAGA,JL,JJ,HW,HW0,R(6),RH2,RCO,
     1               DELH(7),DELH2,DELCO,DELTAZ,RECORE,DENSB,DENSP,
     2               FSTAR,TCORS,TCOR,TANN,GIBB(7),H2OSAT,
     3               KEFF,OPPOSE(9),GASFLO
      DATA ZZ/0.0,0.3,0.6,0.85,0.89,0.93,0.97,1.02,1.07,1.1,1.14,
     1        1.2,1.3/
      DATA DIA1/0.72,0.72,0.72,0.72,0.63,0.54,0.45,0.45,0.45,
     1        0.34,0.20,0.27,0.40/
C-----------------------------------------------------------------------
      IF(Z.NE.0.)GO TO 5
      D1=0.72
      GO TO 40
   5  NPTSG=13
      IF(Z.LT.1.3)GO TO 10
C     ASSUME BED STILL CONFINED RADIALLY TO DIAMETER OF CONE
C     FROM BOTTOM OF CONE TO GRATE LEVEL
      D1=0.40
      GO TO 40
  10  ZDUM=Z
      CALL INTERP(NPTSG,ZZ,DIA1,D1,ZDUM)
  40  RAD0=D1/2.
      RAD1=RAD0+0.01
      RAD2=0.425
      RAD3=RAD2+0.01
      AREA0=3.1416*RAD0**2
      RETURN
      END
```

```
C=======================================================================
      SUBROUTINE AIR(Z)
C=======================================================================
C     THE AMOUNT OF AIR ALLOTTED TO EACH COMPARTMENT IN THE
C     VICINITY OF THE TUYERES IS COMPUTED FROM THE AIR DISTRIBUTION
C     FUNCTION.
C-----------------------------------------------------------------------
      REAL             MIDDLE,KEFF
      DIMENSION        ZDIF(2),EQ(2,2)
      COMMON/GAS    /FAIRIN,EH2O,EO2,EN2,TAIR,PAIR,FAIR,ZL,
     1               ZAIR,WIDTH
      COMMON/LOCAL /IZ,ICOUNT,IFLAGA,JL,JJ,HW,HWO,R(6),RH2,RCO,
     1              DELH(7),DELH2,DELCO,DELTAZ,RECORE,DENSB,DENSP,
     2              FSTAR,TCORS,TCOR,TANN,GIBB(7),H2OSAT,
     3              KEFF,OPPOSE(9),GASFLO
C-----------------------------------------------------------------------
      RETURN
      ZDIF(1)=ABS(Z-ZAIR)
      ZDIF(2)=ABS(Z+DELTAZ-ZAIR)
      IF((ZDIF(1).LE..05385*WIDTH).AND.(ZDIF(2).LE..05385*WIDTH))
     1      GO TO 10
      IF((ZDIF(1).GE..05385*WIDTH).AND.(ZDIF(2).GE..05385*WIDTH))
     1      GO TO 30
      GO TO 60
 10   DO 20 I=1,2
      EQ(1,I)=-199.63*ZDIF(I)/WIDTH+13.1
 20   CONTINUE
      J=1
      GO TO 50
 30   DO 40 I=1,2
      EQ(2,I)=-2.5*ZDIF(I)/WIDTH+2.5
 40   CONTINUE
      J=2
 50   FAIR=(EQ(J,1)+EQ(J,2))/2.*DELTAZ*FAIRIN/(3.0554*WIDTH)
      GO TO 90
 60   IF(ZDIF(1).GT.0.05385*WIDTH)GO TO 70
      L=1
      M=2
      GO TO 80
 70   L=2
      M=1
 80   EQ(1,1)=-199.63*ZDIF(L)/WIDTH+13.1
      EQ(2,2)=-2.5*ZDIF(M)/WIDTH+2.5
      MIDDLE=2.35
      FAIR=((EQ(1,1)+MIDDLE)/2.*(ABS(ZDIF(L)-0.05385*WIDTH))+
     1      (EQ(2,2)+MIDDLE)/2.*(ABS(ZDIF(M)-0.05385*WIDTH)))
     2      *FAIRIN/3.0554/WIDTH
 90   RETURN
      END
```

```
C=====================================================================
      SUBROUTINE INTERP(NPTS,U,V,C,XBAR)
C=====================================================================
C     LINEAR INTERPOLATION AND EXTRAPOLATION
C
      INTEGER I,NPTS
      REAL XBAR,U,V,C
      DIMENSION U(NPTS),V(NPTS)
      IF(XBAR .LT. U(1) ) GO TO 40
      IF(XBAR .GT. U(NPTS)) GO TO 20
      DO 10 I = 1,NPTS
      IF(XBAR .LE. U(I) ) GO TO 60
 10   CONTINUE
 20   WRITE (7,30)
 30   FORMAT('1','XBAR IS BEYOND THE RANGE OF DATA')
      C=V(NPTS-1)-(U(NPTS-1)-XBAR)/(U(NPTS-1)-U(NPTS))*
     1  (V(NPTS-1)-V(NPTS))
      GO TO 80
 40   WRITE (7,50)
 50   FORMAT('0','XBAR IS BELOW THE RANGE OF DATA')
      C=V(2)-(U(2)-XBAR)/(U(2)-U(1))*(V(2)-V(1))
      GO TO 80
 60   IF(XBAR .EQ. U(I)) GO TO 70
      C = V(I-1) + (XBAR-U(I-1))/(U(I)-U(I-1))*(V(I)-V(I-1))
      GO TO 80
 70   C = V(I)
 80   RETURN
      END
```

```
C=======================================================================
      SUBROUTINE EQUIL(Y)
C=======================================================================
C     THIS SUBROUTINE COMPUTES THE POTENTIAL EQUILIBRIUM
C     COMPOSITION OF THE GAS-SOLID MIXTURE AT ANY POINT IN THE
C     GASIFIER.  IF SOLID CHAR IS NOT PRESENT, I.E. ONLY ASH
C     REMAINS, THEN SUBROUTINE EQUILB IS USED INSTEAD.
C-----------------------------------------------------------------------
      REAL           MOLWT,MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,
     1               LAMBDA,KS,NCO,NCO2,NN2,NH2,NH2O,NCH4,NO2,Y(11)
     2               ,A(7,7),B(7,1),WKAREA(20),NC,MOLSC,KEFF,N2
      COMMON/EQUIM /NH2O,NH2,NCH4,NCO,NCO2,NO2,NN2
      COMMON/INPUT /TGUESS,RG,PRESS,TAMB,DP
      COMMON/LOCAL /IZ,ICOUNT,IFLAGA,JL,JJ,HW,HWO,R(6),RH2,RCO,
     1              DELH(7),DELH2,DELCO,DELTAZ,RECORE,DENSB,DENSP,
     2              FSTAR,TCORS,TCOR,TANN,GIBB(7),H2OSAT,
     3              KEFF,OPPOSE(9),GASFLO
      COMMON/PROPS /MOLWT(8),MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,
     1              VISANN,VISCOR,VISAIR,CPAVAN,CPANN(8),CPCOR(9),
     2              CPAIR,DIF(8),DEFF(8),LAMBDA(7),EMISS,COMPN(8),
     3              DENSGC,DENSGA,PP(8),PPEQ(8),CPAVCO,KS
C-----------------------------------------------------------------------
      T=Y(10)
      GASR=1.987
      OE=COMPN(2)+COMPN(5)+2.*COMPN(6)+2.*COMPN(7)
      HE=2.*COMPN(2)+2.*COMPN(3)+4.*COMPN(4)
      TC=COMPN(1)+COMPN(4)+COMPN(5)+COMPN(6)
      IF(ABS(COMPN(7)).LT.1.0E-10)GO TO 10
      CMBCO2=(2.-LAMBDA(3))*COMPN(7)
      CMBCO =2.*(LAMBDA(3)-1.)*COMPN(7)
      C=CMBCO2+CMBCO
      IF(C.GT.COMPN(1))GO TO 40
      NCO=COMPN(5)+CMBCO
      NCO2=COMPN(6)+CMBCO2
      GO TO 15
   10 NCO2=COMPN(6)
      NCO =COMPN(5)
   15 NO2=0.0
      NN2=COMPN(8)
      NH2O=COMPN(2)
      NH2=COMPN(3)
      NCH4=COMPN(4)
      H2O=NH2O
      H2=NH2
      CH4=NCH4
      CO=NCO
      CO2=NCO2
      O2=NO2
      N2=NN2
      IF(NH2O.LE.0.0)NH2O=0.5E-10
      IF(NH2 .LE.0.0)NH2 =0.5E-10
      IF(NCH4.LE.0.0)NCH4=0.5E-10
      IF(NCO .LE.0.0)NCO =0.5E-10
```

```
      IF(NCO2.LE.0.0)NCO2=0.5E-10
      DO 100 ITER=1,50
      TOTAL=NH2O+NH2+NCH4+NCO+NCO2+NN2
      A(1,1)=(TOTAL-NCO2)/NCO2/TOTAL
      A(1,2)=-1.0/TOTAL
      A(1,3)=-1.0/TOTAL
      A(1,4)=-1.0/TOTAL
      A(1,5)=-1.0/TOTAL
      A(1,6)=2.0
      A(1,7)=0.0
      A(2,1)=-1.0/TOTAL
      A(2,2)=(TOTAL-NCO)/NCO/TOTAL
      A(2,3)=-1.0/TOTAL
      A(2,4)=-1.0/TOTAL
      A(2,5)=-1.0/TOTAL
      A(2,6)=1.0
      A(2,7)=0.0
      A(3,1)=-1.0/TOTAL
      A(3,2)=-1.0/TOTAL
      A(3,3)=(TOTAL-NH2O)/NH2O/TOTAL
      A(3,4)=-1.0/TOTAL
      A(3,5)=-1.0/TOTAL
      A(3,6)=1.0
      A(3,7)=1.0
      A(4,1)=-1.0/TOTAL
      A(4,2)=-1.0/TOTAL
      A(4,3)=-1.0/TOTAL
      A(4,4)=(TOTAL-NH2)/NH2/TOTAL
      A(4,5)=-1.0/TOTAL
      A(4,6)=0.0
      A(4,7)=1.0
      A(5,1)=-1.0/TOTAL
      A(5,2)=-1.0/TOTAL
      A(5,3)=-1.0/TOTAL
      A(5,4)=-1.0/TOTAL
      A(5,5)=(TOTAL-NCH4)/NCH4/TOTAL
      A(5,6)=0.0
      A(5,7)=2.0
      DO 20 I=1,7
      A(6,I)=0.0
      A(7,I)=0.0
   20 CONTINUE
      A(6,1)=2.0
      A(6,2)=1.0
      A(6,3)=1.0
      A(7,3)=1.0
      A(7,4)=1.0
      A(7,5)=2.0
      B(1,1)=(TOTAL-NCO2-NCO-NH2O-NH2-NCH4-(TOTAL*GIBB(5)/GASR/T)-
     1       (TOTAL*ALOG(NCO2*PRESS/TOTAL)))/TOTAL
      B(2,1)=(TOTAL-NCO-NCO2-NH2O-NH2-NCH4-(TOTAL*GIBB(4)/GASR/T)-
     1       (TOTAL*ALOG(NCO *PRESS/TOTAL)))/TOTAL
      B(3,1)=(TOTAL-NH2O-NCO2-NCO-NH2-NCH4-(TOTAL*GIBB(1)/GASR/T)-
```

```
     1        (TOTAL*ALOG(NH2O*PRESS/TOTAL)))/TOTAL
      B(4,1)=(TOTAL-NH2-NCO2-NCO-NH2O-NCH4-(TOTAL*GIBB(2)/GASR/T)-
     1        (TOTAL*ALOG(NH2 *PRESS/TOTAL)))/TOTAL
      B(5,1)=(TOTAL-NCH4-NCO2-NCO-NH2O-NH2-(TOTAL*GIBB(3)/GASR/T)-
     1        (TOTAL*ALOG(NCH4*PRESS/TOTAL)))/TOTAL
      B(6,1)=OE
      B(7,1)=HE/2.0
      N=7
      M=1
      IA=7
      IDGT=0
      CALL LINEAR(A,M,N,IA,B,IDGT,WKAREA,IER)
      IF(NCO2.GT.0.1E-7)GO TO 500
92    DFCO2=0.0
      GO TO 510
500   IF(ABS(B(1,1)).LE.0.1E-7)GO TO 92
      DFCO2=ABS(NCO2-B(1,1))
510   IF(NCO.GT.0.1E-7)GO TO 520
512   DFCO=0.0
      GO TO 530
520   IF(ABS(B(2,1)).LE.0.1E-7)GO TO 512
      DFCO=ABS(NCO-B(2,1))
530   IF(NH2O.GT.0.1E-7)GO TO 540
532   DFH2O=0.0
      GO TO 550
540   IF(ABS(B(3,1)).LE.0.1E-7)GO TO 532
      DFH2O=ABS(NH2O-B(3,1))
550   IF(NH2.GT.0.1E-7)GO TO 560
552   DFH2=0.0
      GO TO 570
560   IF(ABS(B(4,1)).LE.0.1E-7)GO TO 552
      DFH2=ABS(NH2-B(4,1))
570   IF(NCH4.GT.0.1E-7)GO TO 580
572   DFCH4=0.0
      GO TO 590
580   IF(ABS(B(5,1)).LE.0.1E-7)GO TO 572
      DFCH4=ABS(NCH4-B(5,1))
590   CONTINUE
      DO 33 II=1,5
      DEC=0.01*ABS(B(II,1))
      GO TO (41,42,43,44,45),II
41    IF(DFCO2.LE.DEC)GO TO 33
      GO TO 47
42    IF(DFCO .LE.DEC)GO TO 33
      GO TO 47
43    IF(DFH2O.LE.DEC)GO TO 33
      GO TO 47
44    IF(DFH2 .LE.DEC)GO TO 33
      GO TO 47
45    IF(DFCH4.LE.DEC)GO TO 33
      GO TO 47
33    CONTINUE
      GO TO 105
```

```
 47   DO 121 IJ=1,7
      IF(B(IJ,1).LE.0.0)B(IJ,1)=0.5E-10
 121  CONTINUE
      NCO2=B(1,1)
      NCO=B(2,1)
      NH2O=B(3,1)
      NH2=B(4,1)
      NCH4=B(5,1)
 100  CONTINUE
      GO TO 115
 105  CONTINUE
C     MOLSC=COMPN(1)
C     QC=MOLSC-COMPN(6)+COMPN(4)-COMPN(5)-2.*COMPN(7)
C     NC=QC+B(1,1)+B(2,1)-B(5,1)
C     MOLSC=NC
C     IF(MOLSC.GT.0.0)GO TO 120
C     MOLSC=0.0
C     WRITE(7,114)
C     WRITE(6,114)
C114  FORMAT(' MOLES OF CARBON IS NEGATIVE THEREFORE ZERO AT EQUIL')
      GO TO 120
 115  WRITE(6,125)ITER
 125  FORMAT(' EQUIL DOES NOT CONVERGE IN ',I3,' ITERATIONS')
 120  CONTINUE
      DO 900 I=1,5
      IF(B(I,1).LT.0.0)B(I,1)=0.0
 900  CONTINUE
      SUM=B(1,1)+B(2,1)+B(3,1)+B(4,1)+B(5,1)+COMPN(8)
      PPEQ(6)=B(1,1)*PRESS/SUM
      PPEQ(5)=B(2,1)*PRESS/SUM
      PPEQ(4)=B(5,1)*PRESS/SUM
      PPEQ(3)=B(4,1)*PRESS/SUM
      PPEQ(2)=B(3,1)*PRESS/SUM
      PPEQ(7)=0.000
      PPEQ(8)=COMPN(8)*PRESS/SUM
      GO TO 999
 90   WRITE(6,91)
 91   FORMAT(' NO SOLID CARBON PRESENT FOR EQUIL')
      PAUSE' CHECK'
      RETURN
 999  C=B(1,1)+B(2,1)+B(5,1)
      IF(C.LE.TC)RETURN
      GO TO 400
 40   CMBCO2=CMBCO2*COMPN(1)/C
      CMBCO =CMBCO *COMPN(1)/C
      NCO2=COMPN(6)+CMBCO2
      NCO =COMPN(5)+CMBCO
      NO2 =COMPN(7)-CMBCO2-0.5*CMBCO
      NH2O=COMPN(2)
      NH2=COMPN(3)
      NCH4=COMPN(4)
      NN2=COMPN(8)
      GO TO 401
```

```
 400  NH2O=H2O
      NH2=H2
      NCH4=CH4
      NCO=CO
      NCO2=CO2
      NO2=O2
      NN2=N2
 401  CALL EQUILB(Y)
C     WRITE(7,4012)PPEQ(2),PPEQ(3),PPEQ(4),PPEQ(5),PPEQ(6),PPEQ(8)
      WRITE(6,4012)PPEQ(2),PPEQ(3),PPEQ(4),PPEQ(5),PPEQ(6),PPEQ(8)
 4012 FORMAT(' PPEQ',6(1X,G10.3))
      RETURN
      END
```

```
C=======================================================================
      SUBROUTINE EQUILB(Y)
C=======================================================================
C     THIS SUBROUTINE IS USED TO COMPUTE THE POTENTIAL EQUILIBRIUM
C     COMPOSITION OF THE GAS-SOLID MIXTURE IN THE GASIFIER WHEN
C     NO REACTIVE CHAR IS PRESENT.
C-----------------------------------------------------------------------
      REAL           MOLWT,MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,
     1               LAMBDA,KS,NCO,NCO2,NN2,NH2,NH2O,NCH4,NO2,Y(11)
     2               ,A(8,8),B(8,1),WKAREA(20),KEFF,N2
      COMMON/EQUIM /NH2O,NH2,NCH4,NCO,NCO2,NO2,NN2
      COMMON/INPUT /TGUESS,RG,PRESS,TAMB,DP
      COMMON/LOCAL /IZ,ICOUNT,IFLAGA,JL,JJ,HW,HWO,R(6),RH2,RCO,
     1              DELH(7),DELH2,DELCO,DELTAZ,RECORE,DENSB,DENSP,
     2              FSTAR,TCORS,TCOR,TANN,GIBB(7),H2OSAT,
     3              KEFF,OPPOSE(9),GASFLO
      COMMON/PROPS /MOLWT(8),MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,
     1              VISANN,VISCOR,VISAIR,CPAVAN,CPANN(8),CPCOR(9),
     2              CPAIR,DIF(8),DEFF(8),LAMBDA(7),EMISS,COMPN(8),
     3              DENSGC,DENSGA,PP(8),PPEQ(8),CPAVCO,KS
C-----------------------------------------------------------------------
      T=Y(10)
      GASR=1.987
      COMBUS=2.*NCH4+0.5*NCO+0.5*NH2
      IF(NO2.LT.COMBUS)GO TO 777
      CH4=0.0
      CO=0.0
      H2=0.0
      O2=NO2-COMBUS
      CO2=NCO2+NCH4+NCO
      H2O=NH2O+NH2+2.*NCH4
      N2=NN2
      NTOT=CO2+CO+H2O+H2+CH4+O2+N2
  100 PPEQ(2)=H2O*PRESS/NTOT
      PPEQ(3)=H2 *PRESS/NTOT
      PPEQ(4)=CH4*PRESS/NTOT
      PPEQ(5)=CO*PRESS/NTOT
      PPEQ(6)=CO2*PRESS/NTOT
      PPEQ(7)=O2 *PRESS/NTOT
      PPEQ(8)=N2*PRESS/NTOT
      RETURN
  777 DFO2=COMBUS-NO2
      IF(DFO2.GT.1.0E-7)GO TO 999
      O2=0.0
      H2=0.0
      CH4=0.0
      COBRN=2.*NO2-0.5*NH2-2.*NCH4
      CO=NCO-COBRN
      CO2=NCO2+NCH4+COBRN
      H2O=NH2O+NH2+2.*NCH4
      N2=NN2
      GO TO 100
  999 IF(NH2O.LT.0.5E-10)NH2O=0.5E-9
```

```
      IF(NH2 .LT.0.5E-10)NH2 =0.5E-9
      IF(NCH4.LT.0.5E-10)NCH4=0.5E-9
      IF(NCO .LT.0.5E-10)NCO =0.5E-9
      IF(NCO2.LT.0.5E-10)NCO2=0.5E-9
      ITER=0
 1000 ITER=ITER+1
 1100 TOTAL=NCO2+NCO+NH2O+NH2+NCH4+NN2
      A(1,1)=(TOTAL-NCO2)/NCO2/TOTAL
      A(1,2)=-1.0/TOTAL
      A(1,3)=-1.0/TOTAL
      A(1,4)=-1.0/TOTAL
      A(1,5)=-1.0/TOTAL
      A(1,6)=1.0
      A(1,7)=0.0
      A(1,8)=2.0
      A(2,1)=-1.0/TOTAL
      A(2,2)=(TOTAL-NCO)/NCO/TOTAL
      A(2,3)=-1.0/TOTAL
      A(2,4)=-1.0/TOTAL
      A(2,5)=-1.0/TOTAL
      A(2,6)=1.0
      A(2,7)=0.0
      A(2,8)=1.0
      A(3,1)=-1.0/TOTAL
      A(3,2)=-1.0/TOTAL
      A(3,3)=(TOTAL-NH2O)/NH2O/TOTAL
      A(3,4)=-1.0/TOTAL
      A(3,5)=-1.0/TOTAL
      A(3,6)=0.0
      A(3,7)=2.0
      A(3,8)=1.0
      A(4,1)=-1.0/TOTAL
      A(4,2)=-1.0/TOTAL
      A(4,3)=-1.0/TOTAL
      A(4,4)=(TOTAL-NH2)/NH2/TOTAL
      A(4,5)=-1.0/TOTAL
      A(4,6)=0.0
      A(4,7)=2.0
      A(4,8)=0.0
      A(5,1)=-1.0/TOTAL
      A(5,2)=-1.0/TOTAL
      A(5,3)=-1.0/TOTAL
      A(5,4)=-1.0/TOTAL
      A(5,5)=(TOTAL-NCH4)/NCH4/TOTAL
      A(5,6)=1.0
      A(5,7)=4.0
      A(5,8)=0.0
      DO 1200 I=1,8
      A(6,I)=0.0
      A(7,I)=0.0
      A(8,I)=0.0
 1200 CONTINUE
      A(6,1)=1.0
```

```
      A(6,2)=1.0
      A(6,5)=1.0
      A(7,3)=2.0
      A(7,4)=2.0
      A(7,5)=4.0
      A(8,1)=2.0
      A(8,2)=1.0
      A(8,3)=1.0
      B(1,1)=(TOTAL-NCO2-NCO-NH2O-NH2-NCH4-(TOTAL*GIBB(5)/GASR/T)
     1       -(TOTAL*ALOG(NCO2*PRESS/TOTAL)))/TOTAL
      B(2,1)=(TOTAL-NCO-NCO2-NH2O-NH2-NCH4-(TOTAL*GIBB(4)/GASR/T)
     1       -(TOTAL*ALOG(NCO *PRESS/TOTAL)))/TOTAL
      B(3,1)=(TOTAL-NH2O-NCO2-NCO-NH2-NCH4-(TOTAL*GIBB(1)/GASR/T)
     1       -(TOTAL*ALOG(NH2O*PRESS/TOTAL)))/TOTAL
      B(4,1)=(TOTAL-NH2-NCO2-NCO-NH2O-NCH4-(TOTAL*GIBB(2)/GASR/T)
     1       -(TOTAL*ALOG(NH2 *PRESS/TOTAL)))/TOTAL
      B(5,1)=(TOTAL-NCH4-NCO2-NCO-NH2O-NH2-(TOTAL*GIBB(3)/GASR/T)
     1       -(TOTAL*ALOG(NCH4*PRESS/TOTAL)))/TOTAL
      B(6,1)=COMPN(1)+COMPN(4)+COMPN(5)+COMPN(6)
      B(7,1)=2.*COMPN(2)+2.*COMPN(3)+4.*COMPN(4)
      B(8,1)=2.*COMPN(6)+COMPN(2)+COMPN(5)+2.*COMPN(7)
      N=8
      M=1
      IA=8
      IDGT=0
      CALL LINEAR(A,M,N,IA,B,IDGT,WKAREA,IER)
C     WRITE(6,1111)
C1111 FORMAT(' EQUILB 1')
C     WRITE(6,1112)NCO2,B(1,1)
C     WRITE(6,1112)NCO,B(2,1)
C     WRITE(6,1112)NH2O,B(3,1)
C     WRITE(6,1112)NH2,B(4,1)
C     WRITE(6,1112)NCH4,B(5,1)
C1112 FORMAT(' N B ',2X,G10.3,2X,G10.3)
      DFCO2=ABS(NCO2-B(1,1))
      DFCO=ABS(NCO-B(2,1))
      DFH2O=ABS(NH2O-B(3,1))
      DFH2=ABS(NH2-B(4,1))
      DFCH4=ABS(NCH4-B(5,1))
      DO 333 II=1,5
  350 DEC=AMAX1(1.0E-8,.001*B(II,1))
      GO TO (410,420,430,440,450),II
  410 IF(DFCO2.LT.DEC)GO TO 333
      GO TO 470
  420 IF(DFCO .LT.DEC)GO TO 333
      GO TO 470
  430 IF(DFH2O.LT.DEC)GO TO 333
      GO TO 470
  440 IF(DFH2 .LT.DEC)GO TO 333
      GO TO 470
  450 IF(DFCH4.LT.0.02*ABS(B(II,1)))GO TO 333
      GO TO 470
  333 CONTINUE
```

```
      GO TO 1050
470   DO 1210 IJ=1,8
      IF(B(IJ,1).LT.0.0)B(IJ,1)=NCH4/1000.
1210  CONTINUE
      NCO2=B(1,1)
      NCO =B(2,1)
      NH2O=B(3,1)
      NH2 =B(4,1)
      NCH4=B(5,1)
      IF(NCO2.LE.0.5E-10)NCO2=0.5E-9
      IF(NCO .LE.0.5E-10)NCO =0.5E-9
      IF(NH2O.LE.0.5E-10)NH2O=0.5E-9
      IF(NH2 .LE.0.5E-10)NH2 =0.5E-9
      IF(NCH4.LE.0.5E-10)NCH4=0.5E-9
      IF((ITER.NE.10).AND.(ITER.NE.19).AND.(ITER.NE.20))GO TO 1041
      WRITE(6,1039)NCO2,NCO,NH2O,NH2,NCH4
1039  FORMAT(' EQUILB',5(2X,G10.3))
1041  IF(ITER.LE.20)GO TO 1000
      GO TO 1150
1050  CONTINUE
      DO 2000 I=1,5
      IF(B(I,1).LE.0.5E-10)B(I,1)=0.5E-9
2000  CONTINUE
      GO TO 1300
1150  WRITE(6,1151)
1151  FORMAT(' EQUILB DOES NOT CONVERGE')
1300  SUM=B(1,1)+B(2,1)+B(3,1)+B(4,1)+B(5,1)+NN2
      PPEQ(2)=B(3,1)*PRESS/SUM
      PPEQ(3)=B(4,1)*PRESS/SUM
      PPEQ(4)=B(5,1)*PRESS/SUM
      PPEQ(5)=B(2,1)*PRESS/SUM
      PPEQ(6)=B(1,1)*PRESS/SUM
      PPEQ(7)=0.0
      PPEQ(8)=NN2*PRESS/SUM
      RETURN
      END
```

```
C=============================================================
      SUBROUTINE TGIBB(Y)
C=============================================================
C     THE GIBB'S FREE ENERGY IS COMPUTED FOR EACH COMPONENT AS A
C     FUNCTION OF TEMPERATURE  FOR USE IN THE EQUILIBRIUM
C     CALCULATION.
C-------------------------------------------------------------
      REAL          MOLWT,MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,
     1              LAMBDA,KEFF,KS,MWW(6)
      DIMENSION Y(11),DH(6),DG(6),ALPHA(8),BETA(8),GAMMA(8),DELTA(8),
     1          CF(6,3),ALPHAE(6),BETAE(6),GAMMAE(6),DELTAE(6),
     2          CONST1(6),CONST2(6),CONST3(6),CONST4(6),
     3          DELGF1(6),DELGF2(6)
C     COMMON/INPUT /TGUESS,RG,PRESS,TAMB,DP
      COMMON/LOCAL /IZ,ICOUNT,IFLAGA,JL,JJ,HW,HWO,R(6),RH2,RCO,
     1              DELH(7),DELH2,DELCO,DELTAZ,RECORE,DENSB,DENSP,
     2              FSTAR,TCORS,TCOR,TANN,GIBB(7),H2OSAT,
     3              KEFF,OPPOSE(9),GASFLO
C     COMMON/PROPS /MOLWT(8),MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,
C    1              VISANN,VISCOR,VISAIR,CPAVAN,CPANN(8),CPCOR(9),
C    2              CPAIR,DIF(8),DEFF(8),LAMBDA(7),EMISS,COMPN(8),
C    3              DENSGC,DENSGA,PP(8),PPEQ(8),CPAVCO,KS
      DATA ALPHA/.112990,.252953,.432770,3.33912,.198195,.303762,
     1          .257009,0.0/
      DATA BETA /3.67375E-4,-5.23931E-5,-9.88213E-6,3.80348E-4,
     1          6.69130E-5,6.71565E-4,-6.85723E-5,0.0/
      DATA GAMMA/-2.52036E-7,1.42227E-7,1.92278E-7,-3.91955E-7,
     1          1.44499E-8,3.41444E-7,1.49874E-7,0.0/
      DATA DELTA/6.64461E-11,-5.95073E-11,-6.82349E-11,2.49811E-10,
     1          -1.87652E-11,-2.45482E-10,-5.92428E-11,0.0/
      DATA MWW  /44.01,28.01,18.0153,2.0158,31.9988,16.04/
C-------------------------------------------------------------
      T=Y(10)
      DH(1)=-94051.*4.184
      DH(2)=-26416.*4.184
      DH(3)=-57798.*4.184
      DH(6)=-17889.*4.184
      DG(1)=-94258.
      DG(2)=-32781.
      DG(3)=-54635.
      DG(6)=-12140.
      CF(1,1)=1.0
      CF(1,2)=0.0
      CF(1,3)=1.0
      CF(2,1)=1.0
      CF(2,2)=0.0
      CF(2,3)=0.5
      CF(3,1)=0.0
      CF(3,2)=1.0
      CF(3,3)=0.5
      CF(6,1)=1.0
      CF(6,2)=2.0
      CF(6,3)=0.0
```

```
      DO 10 I=1,6
      ALPHAE(I)=ALPHA(I)*4.184*MWW(I)
      BETAE (I)=BETA (I)*4.184*MWW(I)
      GAMMAE(I)=GAMMA(I)*4.184*MWW(I)
      DELTAE(I)=DELTA(I)*4.184*MWW(I)
10    CONTINUE
      ALPHAC= 4.03    *4.184
      BETAC= 1.14E-3 *4.184
      SIGMAC=-2.04E5 *4.184
      CPC1=(ALPHAC*298.0)+(BETAC*(298.0**2)/2.0)-(SIGMAC/298.0)
      CPC2=(ALPHAC*T*ALOG(T))+(BETAC*T**2)/2.0+(SIGMAC/T/2.0)
      CPC3=(ALPHAC*ALOG(298.))+(BETAC*298./2.0)+(SIGMAC/(298.**2)/2.0)
      DO 20 I=1,6
      CONST1(I)=(ALPHAE(I)*298.)+(BETAE(I)*298.**2)/2.0+
     1          (GAMMAE(I)*298.**3)/3.0+(DELTAE(I)*298.**4)/4.0
20    CONTINUE
      DO 30 J=1,6
      IF(J.LE.3)GO TO 22
      IF(J.EQ.4)GO TO 23
      GO TO 30
22    I=J
      GO TO 25
23    I=6
25    CONST2(I)=CONST1(I)-CF(I,1)*CPC1-CF(I,2)*CONST1(4)-
     1          CF(I,3)*CONST1(5)
30    CONTINUE
      DO 40 I=1,6
      CONST3(I)=(ALPHAE(I)*T*ALOG(T))+(BETAE(I)*T**2)/2.0
     1         +(GAMMAE(I)*T**3)/6.0 +(DELTAE(I)*T**4)/12.0
40    CONTINUE
      DO 50 J=1,6
      IF(J.LE.3)GO TO 35
      IF(J.EQ.4)GO TO 33
      GO TO 50
35    I=J
      GO TO 37
33    I=6
37    DELGF1(I)=(-1.*CONST3(I))+(CF(I,1)*CPC2)+(CF(I,2)*CONST3(4))
     1          +(CF(I,3)*CONST3(5))+DH(I)-CONST2(I)
50    CONTINUE
      DO 60 I=1,6
      CONST4(I)=(ALPHAE(I)*ALOG(298.))+(BETAE(I)*298./2.0)
     1        +(GAMMAE(I)*298.**2)/6.0+(DELTAE(I)*298.**3)/12.0
60    CONTINUE
      DO 70 J=1,6
      IF(J.LE.3)GO TO 64
      IF(J.EQ.4)GO TO 62
      GO TO 70
64    I=J
      GO TO 66
62    I=6
66    DELGF2(I)=CONST4(I)-CF(I,1)*CPC3-CF(I,2)*CONST4(4)-
     1         CF(I,3)*CONST4(5)-DH(I)/298.+CONST2(I)/298.
```

```
70    CONTINUE
      GIBB(5)=(DELGF1(1)+T*DELGF2(1))/4.184+T/298.*DG(1)
      GIBB(4)=(DELGF1(2)+T*DELGF2(2))/4.184+T/298.*DG(2)
      GIBB(1)=(DELGF1(3)+T*DELGF2(3))/4.184+T/298.*DG(3)
      GIBB(3)=(DELGF1(6)+T*DELGF2(6))/4.184+T/298.*DG(6)
      GIBB(2)=0.0
      GIBB(6)=0.0
      GIBB(7)=0.0
      RETURN
      END
```

```
C=======================================================================
      SUBROUTINE LINEAR(A,M,N,IA,B,IDGT,WKAREA,IER)
C=======================================================================
C     SEE IMSL SUBROUTINE LEQT1F
C-----------------------------------------------------------------------
      DIMENSION  A(N,N),B(N,M),WKAREA(20)
      IER=0
      CALL LUDATF (A,A,N,IA,IDGT,D1,D2,WKAREA,WKAREA,WA,IER)
      IF(IER.GT.128)GO TO 10
      CALL LUELMF (A,B,WKAREA,N,IA,B)
      IF(IER.EQ.0)GO TO 20
 10   CONTINUE
      CALL UERTST (IER,6HLINEAR)
 20   RETURN
      END
```

```
C=======================================================================
      SUBROUTINE FCNJ(N,Z,Y,YPRIME)
C=======================================================================
      INTEGER N
      REAL Y(N),YPRIME(N)
      RETURN
      END
```

```
C=======================================================================
      SUBROUTINE READIN
C=======================================================================
C     THIS SUBROUTINE CONTROLS READING OF THE INPUT DATA FROM A
C     FILE INPUT.DAT.
C-----------------------------------------------------------------------
      REAL           KEFF
      COMMON/ANALYS/ANALA,ANALC,ANALH,ANALN,ANALO,PROXW,PROXC,
     1              PROXV,PROXA,PMOLO,PMOLC,PMOLH,EMAS(6),HCOMBW
      COMMON/INDATA/METH1,METH2,METH3,MITER1,MITER2,MITER3,H1,H2,
     1              H3,TOL,ITERAT
      COMMON/GAS   /FAIRIN,EH2O,EO2,EN2,TAIR,PAIR,FAIR,
     1              ZL,ZAIR,WIDTH
      COMMON/LOCAL /IZ,ICOUNT,IFLAGA,JL,JJ,HW,HWO,R(6),RH2,RCO,
     1              DELH(7),DELH2,DELCO,DELTAZ,RECORE,DENSB,DENSP,
     2              FSTAR,TCORS,TCOR,TANN,GIBB(7),H2OSAT,
     3              KEFF,OPPOSE(9),GASFLO
      COMMON/INPUT /TGUESS,RG,PRESS,TAMB,DP
      COMMON/WOOD  /FSO,DL,DH,DW,VOIDP,VOID,DENSBO,DENSPO
C-----------------------------------------------------------------------
      READ(5,10)FSO,DENSPO,DENSBO
      READ(5,20)DL,DH,DW,VOIDP
      READ(5,30)PROXC,PROXW,PROXV,PROXA
      READ(5,40)ANALA,ANALC,ANALH,ANALN,ANALO
      READ(5,50)FAIRIN,TAIR,PAIR
      READ(5,60)EH2O,EO2,EN2
      READ(5,70)WIDTH
      READ(5,80)TAMB
      READ(5,90)ZL,ZAIR,PRESS
      READ(5,100)METH1,MITER1
      READ(5,100)METH2,MITER2
      READ(5,100)METH3,MITER3
      READ(5,110)TOL
      READ(5,120)IZ,ITERAT
      READ(5,130)H1,H2,H3
      READ(5,140)TGUESS
 10   FORMAT(T7,F6.4,T15,F6.1,T23,F6.1)
 20   FORMAT(T7,F5.3,T15,F5.3,T23,F5.3,T31,F4.2)
 30   FORMAT(T7,F6.4,T15,F6.4,T23,F6.4,T31,F6.4)
 40   FORMAT(T7,F6.4,T15,F6.4,T23,F6.4,T31,F6.4,T39,F6.4)
 50   FORMAT(T7,F5.3,T15,F4.0,T23,F5.1)
 60   FORMAT(T7,F5.3,T15,F5.3,T23,F5.3)
 70   FORMAT(T7,F5.3)
 80   FORMAT(T7,F5.0)
 90   FORMAT(T7,F4.2,T15,F4.2,T23,F5.1)
 100  FORMAT(T7,I1,T15,I1)
 110  FORMAT(T7,E10.1)
 120  FORMAT(T7,I4,T15,I3)
 130  FORMAT(T7,F7.5,T15,F7.5,T23,F7.5)
 140  FORMAT(T7,F5.0)
      RETURN
      END
```

```
C=============================================================
      SUBROUTINE OUTPUT
C=============================================================
C     THIS FILE CONTAINS THE FORMATTING REQUIRED FOR THE FINAL
C     OUTPUT DATA FROM THE SIMULATION.
C-------------------------------------------------------------
      REAL           K7,MOLWT,MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,
     1               LAMBDA,MASBAL,KEFF,KS,
     2               NH2O,NH2,NCH4,NCO,NCO2,NO2,NN2
      REAL           PROF1(100),PROF2(100),PROF3(100),PROF4(100),
     1               PROF5(100),PROF6(100),PROF7(100),PROF8(100),
     2               PROF9(100),PROF10(100)
      COMMON/ANALYS/ANALA,ANALC,ANALH,ANALN,ANALO,PROXW,PROXC,
     1               PROXV,PROXA,PMOLO,PMOLC,PMOLH,EMAS(6),HCOMBW
      COMMON/DIMENS/RAD0,RAD1,RAD2,RAD3,AREA0
      COMMON/GAS    /FAIRIN,EH2O,EO2,EN2,TAIR,PAIR,FAIR,
     1               ZL,ZAIR,WIDTH
      COMMON/INPUT  /TGUESS,RG,PRESS,TAMB,DP
      COMMON/LOCAL  /IZ,ICOUNT,IFLAGA,JL,JJ,HW,HW0,R(6),RH2,RCO,
     1               DELH(7),DELH2,DELCO,DELTAZ,RECORE,DENSB,DENSP,
     2               FSTAR,TCORS,TCOR,TANN,GIBB(7),H2OSAT,
     3               KEFF,OPPOSE(9),GASFLO
      COMMON/PROFIL/PROF1,PROF2,PROF3,PROF4,PROF5,PROF6,PROF7,
     1               PROF8,PROF9,PROF10
      COMMON/PROPS  /MOLWT(8),MWAVA,MWAVC,MWAIR,KGANN,KGCOR,KAIR,
     1               VISANN,VISCOR,VISAIR,CPAVAN,CPANN(8),CPCOR(9),
     2               CPAIR,DIF(8),DEFF(8),LAMBDA(7),EMISS,COMPN(8),
     3               DENSGC,DENSGA,PP(8),PPEQ(8),CPAVCO,KS
      COMMON/WOOD   /FS0,DL,DH,DW,VOIDP,VOID,DENSB0,DENSP0
C-------------------------------------------------------------
      WRITE(6,10)
 10   FORMAT(' ',65('='),/,
     1'      SIMULATION OF DOWN DRAFT WOOD GASIFIER OPERATION',/,
     2'                 DEPT. OF CHEMICAL ENGINEERING        ',/,
     3'                       QUEEN''S UNIVERSITY            ',/,
     4'                            1981-1983                 ',/,
     5       65('='),/)
      WRITE(6,20)
 20   FORMAT(' ',5X,'RUN NO.:',          /,
     1           6X,'DATE   :',          /,
     2           6X,'TIME   :',           )
C-------------------------------------------------------------
C     INPUT DATA
      RATIO=FAIRIN/FS0
      FS0=FS0*3600.
      FAIRIN=FAIRIN*3600.
      PAIR=PAIR*101.325
      DL=DL*2.
      WRITE(6,30)FS0,FAIRIN,DENSP0,TAIR,DENSB0,PAIR,DL,RATIO
 30   FORMAT(' ',5X,'INPUT DATA',/,
     1           6X,'WOOD RATE  (KG/HR): ',F6.1,3X,
     2              'AIR  RATE  (KG/HR): ',F6.1,/,
     3           6X,'WOOD DENS  (KG/M3): ',F6.1,3X,
```

```
     4              'AIR  TEMP  (K)    : ',F6.1,/,
     5           6X,'BED  DENS  (KG/M3): ',F6.1,3X,
     6              'AIR  PRES  (KPA)  : ',F6.2,/,
     7           6X,'WOOD SIZE  (M)    : ',F6.2,3X,
     8              'RATIO  (AIR/WOOD) : ',F5.3,/,
     9           65('='),/)
      WRITE(6,40)ZL,TGUESS,ZAIR,PRESS,WIDTH,TAMB
 40   FORMAT(' ',5X,'BED HEIGHT   (M): ',F4.2,
     1          T30,'TEMP GUESS   (K): ',F4.0,/,
     2           6X,'TUYERE LEVEL (M): ',F4.2,
     3          T30,'BED PRESS  (KPA): ',F6.2,/,
     4           6X,'COMB ZONE    (M): ',F4.2,
     5          T30,'AMBIENT TEMP (K): ',F4.0,/)
      WRITE(6,50)PROXW,ANALC,PROXC,ANALH,PROXV,ANALO,PROXA,ANALN
 50   FORMAT(' ',65('='),/,T5,'PROXIMATE (WT%)',T30,'ULTIMATE (WT%)',
     1                    T55,'AIR (WT%)',/,
     2  T5,'MOISTURE (WB): ',F4.1,T30,'C : ',F5.2,T55,'H2O :',F5.2,/,
     3  T5,'FIXED C  (DB): ',F4.1,T30,'H : ',F5.2,T55,'O2  :',F5.2,/,
     4  T5,'VOLATILE (DB): ',F4.1,T30,'O : ',F5.2,T55,'N2  :',F5.2,/,
     5  T5,'ASH      (DB): ',F4.1,T30,'N : ',F5.2,T55,/)
      WRITE(6,60)METH,H,MITER,IZ,TOL,JJ,ITERAT
 60   FORMAT(' ',5X,'METHOD           : ',I1,
     1          T30,'Z INCREMENT     : ',E12.4,/,
     2           6X,'MITER           : ',I1,
     3          T30,'# COMPARTMENTS  : ',I4,/,
     4           6X,'TOLERANCE       : ',E12.4,
     5          T30,'REQ''D ITERATIONS:',I4,/,
     6          T30,'MAX ITERATIONS  : ',I4,/)
C-----------------------------------------------------------------
C     OUTPUT - PRODUCT GAS AND MEASURE OF PERFORMANCE
      CCONV=MOLWT(1)*(PROF4(JL)/MOLWT(4)+
     1      PROF5(JL)/MOLWT(5)+PROF6(JL)/MOLWT(6))
     2      /(FS0*(1.-PROXW)*ANALC)*100.
      FGAS=PROF2(JL)+PROF3(JL)+PROF4(JL)+PROF5(JL)+PROF6(JL)+
     1     PROF7(JL)+PROF8(JL)
      FASH=PROF1(IZ/2)
      MASBAL=(FGAS+FASH)/(FS0+FAIRIN)*100.
      HHV=-(PROF3(JL)*68317./MOLWT(3)+
     1      PROF4(JL)*212800./MOLWT(4)+
     2      PROF5(JL)*67636./MOLWT(5))*4.184/(FGAS/MWAVA)
     3      /8.205E-5/298
      T=PROF10(JL)
      HGAS1 =PROF2(JL)/MOLWT(2)*
     1            (7.30*T+1.23E-3*T**2-2284.63)
     2           + PROF3(JL)/MOLWT(3)*
     3            (6.52*T+0.39E-3*T**2-0.12E5/T-1937.33)
     4           + PROF4(JL)/MOLWT(4)*
     5            (3.381*T+9.022E-3*T**2-1.433E-6*T**3-1770.80)
     6           + PROF5(JL)/MOLWT(5)*
     7            (6.79*T+0.49E-3*T**2+0.11E5/T-2103.85)
      HGAS2 =PROF6(JL)/MOLWT(6)*
     1            (10.57*T+1.05E-3*T**2+2.06E5/T-3934.38)
     2           + PROF7(JL)/MOLWT(7)*
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     3            (7.16*T+0.5E-3*T**2+0.40E5/T-2312.31)
     4          + PROF8(JL)/MOLWT(8)*
     5            (6.83*T+0.45E-3*T**2+0.12E5/T-2115.57)
      HGAS=4184.*(HGAS1+HGAS2)
      HAIR=4184.*FAIRIN*
     1       (EO2*(7.16*T+0.5E-3*T**2+0.40E5/T-2312.31)+
     2        EN2*(6.83*T+0.45E-3*T**2+0.12E5/T-2115.57)+
     3       EH2O*(7.30*T+1.23E-3*T**2-2284.63))
      TRMEFF=HGAS/(HCOMBW+HAIR)*100.
      WRITE(6,70)FGAS,NH2O,TGAS,NH2,PRESS,NCH4,HHV,NCO,NCO2,FASH,
     1           NO2,CASH,NN2
 70   FORMAT('1',34X,'PRODUCT GAS COMPOSITION',/,
     1   5X,'GAS RATE (KG/HR) : ',F5.1,T40,'H2O    :  ',F5.3,/,
     2   5X,'GAS TEMP     (K) : ',F5.1,T40,'H2     :  ',F5.3,/,
     3   5X,'GAS PRES   (KPA) : ',F5.1,T40,'CH4    :  ',F5.3,/,
     4   5X,'GAS HHV  (KJ/M3) : ',F7.1,T40,'CO     :  ',F5.3,/,
     5   T40,                          'CO2    :  ',F5.3,/,
     6   5X,'ASH PROD (KG/HR) : ',F5.2,T40,'O2     :  ',F5.3,/,
     7   5X,'C IN ASH   (WT%) : ',F5.2,T40,'N2     :  ',F5.3,/,
     8   65('='))
      WRITE(6,90)CCONV,MASBAL,HHV,TRMEFF
 90   FORMAT(' ',5X,'CARBON CONVRSN % :',F6.2,
     1          T30,'HHV OF GAS (J/M3):',F11.2,/,
     2           6X,'MASS BALANCE   % :',F6.2,
     3          T30,'THERMAL EFF    % :',F6.2,/)
C-----------------------------------------------------------------
C     OUTPUT - FINAL COMPOSITION AND TEMPERATURE PROFILES
      WRITE(6,100)
 100  FORMAT(' ','FINAL PROFILES',/,1X,
     1           'ZONE LEVEL  TEMP    C      H2O      H2',
     2       T43,'CH4      CO     CO2      O2      N2',/,
     3       T8,'(M)',T15,'(K)',T47,'(KG/HR)',/,65('='),/)
      DO 130 JJK=1,JL
      WRITE(6,110)ZONE,Z,PROF1(JJK),PROF2(JJK),PROF3(JJK),PROF4(JJK),
     1       PROF5(JJK),PROF6(JJK),PROF7(JJK),PROF8(JJK),PROF9(JJK),
     2       PROF10(JJK)
 110  FORMAT(' ',A4,T7,F5.3,T14,F4.0,T20,F5.3,T27,F5.3,T34,F5.3,
     1           T41,F5.3,T48,F5.3,T55,F5.3,T62,F5.3,T69,F5.3,/)
 130  CONTINUE
C-----------------------------------------------------------------
C     OUTPUT - INTERMEDIATE ITERATION PROFILES
      WRITE(6,140)
 140  FORMAT('1','INTERMEDIATE ITERATION PROFILES',/,65('='),/)
      DO 200 IJK=1,JJ
      WRITE(6,150)IJK
 150  FORMAT(' ','ITERATION # : ',/)
      WRITE(6,160)
 160  FORMAT('1','ZONE LEVEL  TEMP    C      H2O      H2',
     1       T43,'CH4      CO     CO2      O2      N2',/,
     2       T8,'(M)',T15,'(K)',T47,'(KG/HR)',/,65('='),/)
      DO 190 IJL=1,JL
      WRITE(6,170)ZONE,Z,PROF1(IJL),PROF2(IJL),PROF3(IJL),PROF4(IJL),
     1       PROF5(IJL),PROF6(IJL),PROF7(IJL),PROF8(IJL),PROF9(IJL),
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     2         PROF10(IJL)
 170  FORMAT(' ',A4,T7,F5.3,T14,F4.0,T20,F5.3,T27,F5.3,T34,F5.3,
     1           T41,F5.3,T48,F5.3,T55,F5.3,T62,F5.3,T69,F5.3,/)
 190  CONTINUE
 200  CONTINUE
C-----------------------------------------------------------------
      RETURN
      END
```

```
C    IMSL ROUTINE NAME   - DGEAR
C
C-----------------------------------------------------------------------
C
C    COMPUTER            - BGH/SINGLE
C
C    LATEST REVISION     - NOVEMBER 1, 1979
C
C    PURPOSE             - DIFFERENTIAL EQUATION SOLVER - VARIABLE ORDER
C                          ADAMS PREDICTOR CORRECTOR METHOD OR
C                          GEARS METHOD
C
C    USAGE               - CALL DGEAR (N,FCN,FCNJ,X,H,Y,XEND,TOL,METH,
C                          MITER,INDEX,IWK,WK,IER)
C
C    ARGUMENTS    N      - INPUT NUMBER OF FIRST-ORDER DIFFERENTIAL
C                          EQUATIONS. N CAN BE REDUCED, BUT NEVER
C                          INCREASED, DURING A PROBLEM. N MUST BE
C                          GREATER THAN ZERO.
C                 FCN    - NAME OF SUBROUTINE FOR EVALUATING FUNCTIONS.
C                          (INPUT)
C                          THE SUBROUTINE ITSELF MUST ALSO BE PROVIDED
C                            BY THE USER AND IT SHOULD BE OF THE
C                            FOLLOWING FORM
C                              SUBROUTINE FCN (N,X,Y,YPRIME)
C                              REAL Y(N),YPRIME(N)
C                                    .
C                                    .
C                                    .
C                          FCN SHOULD EVALUATE YPRIME(1),...,YPRIME(N)
C                            GIVEN N,X, AND Y(1),...,Y(N). YPRIME(I)
C                            IS THE FIRST DERIVATIVE OF Y(I) WITH
C                            RESPECT TO X.
C                          FCN MUST APPEAR IN AN EXTERNAL STATEMENT IN
C                            THE CALLING PROGRAM AND N,X,Y(1),...,Y(N)
C                            MUST NOT BE ALTERED BY FCN.
C                 FCNJ   - NAME OF THE SUBROUTINE FOR COMPUTING THE N BY
C                          N JACOBIAN MATRIX OF PARTIAL DERIVATIVES.
C                          (INPUT)
C                          THE SUBROUTINE ITSELF MUST ALSO BE PROVIDED
C                            BY THE USER AND IT SHOULD BE OF THE
C                            FOLLOWING FORM
C                              SUBROUTINE FCNJ (N,X,Y,PD)
C                              REAL Y(N),PD(N,N)
C                                    .
C                                    .
C                                    .
C                          FCNJ SHOULD COMPUTE PD(I,J) WHICH IS THE
C                            PARTIAL DERIVATIVE OF YPRIME(I) WITH
C                            RESPECT TO Y(J).
C                          FCNJ MUST APPEAR IN AN EXTERNAL STATEMENT IN
C                            THE CALLING PROGRAM AND N,X,Y(1),...,Y(N)
C                            MUST NOT BE ALTERED BY FCNJ.
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C                 FCNJ IS CALLED ONLY IF MITER IS EQUAL TO
C                   ONE. OTHERWISE A DUMMY ROUTINE CAN BE
C                   SUBSTITUTED. SEE REMARKS.
C       X       - INDEPENDENT VARIABLE. (INPUT AND OUTPUT)
C                   ON INPUT, X SUPPLIES THE INITIAL VALUE AND
C                   AND IS USED ONLY ON THE FIRST CALL.
C                   ON OUTPUT, X IS REPLACED WITH THE CURRENT
C                   VALUE OF THE INDEPENDENT VARIABLE AT WHICH
C                   INTEGRATION HAS BEEN COMPLETED.
C       H       - INPUT/OUTPUT.
C                   ON INPUT, H CONTAINS THE NEXT STEP SIZE IN
C                   X. H IS USED ONLY ON THE FIRST CALL.
C                   ON OUTPUT, H CONTAINS THE STEP SIZE USED
C                   LAST, WHETHER SUCCESSFULLY OR NOT.
C       Y       - DEPENDENT VARIABLES, VECTOR OF LENGTH N.
C                   (INPUT AND OUTPUT)
C                   ON INPUT, Y(1),...,Y(N) SUPPLY INITIAL
C                   VALUES.
C                   ON OUTPUT, Y(1),...,Y(N) ARE REPLACED WITH
C                   A COMPUTED VALUE AT XEND.
C       XEND    - INPUT VALUE OF X AT WHICH SOLUTION IS DESIRED
C                   NEXT. INTEGRATION WILL NORMALLY GO SLIGHTLY
C                   BEYOND XEND AND THE ROUTINE WILL INTERPOLATE
C                   TO X = XEND.
C                 NOTE THAT (X-XEND)*H MUST BE LESS THAN
C                   ZERO (X AND H AS SPECIFIED ON INPUT).
C       TOL     - INPUT RELATIVE ERROR BOUND. TOL MUST BE
C                   GREATER THAN ZERO. TOL IS USED ONLY ON THE
C                   FIRST CALL UNLESS INDEX IS EQUAL TO -1.
C                   TOL SHOULD BE AT LEAST AN ORDER OF
C                   MAGNITUDE LARGER THAN THE UNIT ROUNDOFF
C                   BUT GENERALLY NOT LARGER THAN .001.
C                   SINGLE STEP ERROR ESTIMATES DIVIDED BY
C                   YMAX(I) WILL BE KEPT LESS THAN TOL IN
C                   ROOT-MEAN-SQUARE NORM (EUCLIDEAN NORM
C                   DIVIDED BY SQRT(N)). THE VECTOR YMAX OF
C                   WEIGHTS IS COMPUTED INTERNALLY AND STORED
C                   IN WORK VECTOR WK. INITIALLY YMAX(I) IS
C                   THE ABSOLUTE VALUE OF Y(I), WITH A DEFAULT
C                   VALUE OF ONE IF Y(I) IS EQUAL TO ZERO.
C                   THEREAFTER, YMAX(I) IS THE LARGEST VALUE
C                   OF THE ABSOLUTE VALUE OF Y(I) SEEN SO FAR,
C                   OR THE INITIAL VALUE OF YMAX(I) IF THAT IS
C                   LARGER.
C       METH    - INPUT BASIC METHOD INDICATOR.
C                   USED ONLY ON THE FIRST CALL UNLESS INDEX IS
C                   EQUAL TO -1.
C                 METH = 1, IMPLIES THAT THE ADAMS METHOD IS
C                   TO BE USED.
C                 METH = 2, IMPLIES THAT THE STIFF METHODS OF
C                   GEAR, OR THE BACKWARD DIFFERENTIATION
C                   FORMULAE ARE TO BE USED.
C       MITER   - INPUT ITERATION METHOD INDICATOR.
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C                    MITER = 0, IMPLIES THAT FUNCTIONAL
C                      ITERATION IS USED. NO PARTIAL
C                      DERIVATIVES ARE NEEDED. A DUMMY FCNJ
C                      CAN BE USED.
C                    MITER = 1, IMPLIES THAT THE CHORD METHOD
C                      IS USED WITH AN ANALYTIC JACOBIAN. FOR
C                      THIS METHOD, THE USER SUPPLIES
C                      SUBROUTINE FCNJ.
C                    MITER = 2, IMPLIES THAT THE CHORD METHOD
C                      IS USED WITH THE JACOBIAN CALCULATED
C                      INTERNALLY BY FINITE DIFFERENCES.
C                      A DUMMY FCNJ CAN BE USED.
C                    MITER = 3, IMPLIES THAT THE CHORD METHOD
C                      IS USED WITH THE JACOBIAN REPLACED BY
C                      A DIAGONAL APPROXIMATION BASED ON A
C                      DIRECTIONAL DERIVATIVE.
C                      A DUMMY FCNJ CAN BE USED.
C               INDEX  - INPUT AND OUTPUT PARAMETER USED TO INDICATE
C                      THE TYPE OF CALL TO THE SUBROUTINE.
C                    ON INPUT, INDEX = 1, IMPLIES THAT THIS IS THE
C                      FIRST CALL FOR THIS PROBLEM. ON OUTPUT INDEX
C                      IS RESET TO 0 IF INTEGRATION WAS SUCCESSFUL.
C                      OTHERWISE, THE VALUE OF INDEX IS UNCHANGED.
C                    ON INPUT, INDEX = 0, IMPLIES THAT THIS IS NOT
C                      THE FIRST CALL FOR THIS PROBLEM. INDEX IS
C                      UNCHANGED ON OUTPUT.
C                    ON INPUT, INDEX = -1, IMPLIES THAT THIS IS NOT
C                      THE FIRST CALL FOR THIS PROBLEM, AND THE
C                      USER HAS RESET TOL. ON OUTPUT INDEX IS RESET
C                      TO 0 IF INTEGRATION WAS SUCCESSFUL.
C                      OTHERWISE THE VALUE OF INDEX IS UNCHANGED.
C                    ON INPUT, INDEX = 2, IMPLIES THAT THIS IS NOT
C                      THE FIRST CALL FOR THIS PROBLEM. INTEGRATION
C                      IS TO CONTINUE AND XEND IS TO BE HIT EXACTLY
C                      (NO INTERPOLATION IS DONE). THIS VALUE OF
C                      INDEX ASSUMES THAT XEND IS BEYOND THE
C                      CURRENT VALUE OF X. INDEX IS UNCHANGED ON
C                      OUTPUT.
C                    ON INPUT, INDEX = 3, IMPLIES THAT THIS IS NOT
C                      THE FIRST CALL FOR THIS PROBLEM. INTEGRATION
C                      IS TO CONTINUE AND CONTROL IS TO BE RETURNED
C                      TO THE CALLING PROGRAM AFTER ONE STEP. XEND
C                      IS IGNORED. INDEX IS UNCHANGED ON OUTPUT.
C               IWK    - INTEGER WORK VECTOR OF LENGTH N. USED ONLY IF
C                      MITER IS EQUAL TO 1 OR 2.
C               WK     - REAL WORK VECTOR OF LENGTH 4*N+NMETH+NMITER.
C                      THE VALUE OF NMETH DEPENDS ON THE VALUE OF
C                        METH.
C                        IF METH IS EQUAL TO 1,
C                          NMETH IS EQUAL TO N*13.
C                        IF METH IS EQUAL TO 2,
C                          NMETH IS EQUAL TO N*6.
C                      THE VALUE OF NMITER DEPENDS ON THE VALUE OF
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C                          MITER.
C                          IF MITER IS EQUAL TO 1 OR 2,
C                            NMITER IS EQUAL TO N*(N+1).
C                          IF MITER IS EQUAL TO 3,
C                            NMITER IS EQUAL TO N.
C                          IF MITER IS EQUAL TO 0,
C                            NMITER IS EQUAL TO 1.
C                        WK MUST REMAIN UNCHANGED BETWEEN SUCCESSIVE
C                        CALLS DURING INTEGRATION.
C                IER   - ERROR PARAMETER. (OUTPUT)
C                        WARNING ERROR
C                          IER = 33, IMPLIES THAT X+H WILL EQUAL X ON
C                            THE NEXT STEP. THIS CONDITION DOES NOT
C                            FORCE THE ROUTINE TO HALT. HOWEVER, IT
C                            DOES INDICATE ONE OF TWO CONDITIONS.
C                            THE USER MIGHT BE REQUIRING TOO MUCH
C                            ACCURACY VIA THE INPUT PARAMETER TOL.
C                            IN THIS CASE THE USER SHOULD CONSIDER
C                            INCREASING THE VALUE OF TOL. THE OTHER
C                            CONDITION WHICH MIGHT GIVE RISE TO THIS
C                            ERROR MESSAGE IS THAT THE SYSTEM OF
C                            DIFFERENTIAL EQUATIONS BEING SOLVED
C                            IS STIFF (EITHER IN GENERAL OR OVER
C                            THE SUBINTERVAL OF THE PROBLEM BEING
C                            SOLVED AT THE TIME OF THE ERROR). IN
C                            THIS CASE THE USER SHOULD CONSIDER
C                            USING A NONZERO VALUE FOR THE INPUT
C                            PARAMETER MITER.
C                        WARNING WITH FIX ERROR
C                          IER = 66, IMPLIES THAT THE ERROR TEST
C                            FAILED. H WAS REDUCED BY .1 ONE OR MORE
C                            TIMES AND THE STEP WAS TRIED AGAIN
C                            SUCCESSFULLY.
C                          IER = 67, IMPLIES THAT CORRECTOR
C                            CONVERGENCE COULD NOT BE ACHIEVED.
C                            H WAS REDUCED BY .1 ONE OR MORE TIMES AND
C                            THE STEP WAS TRIED AGAIN SUCCESSFULLY.
C                        TERMINAL ERROR
C                          IER = 132, IMPLIES THE INTEGRATION WAS
C                            HALTED AFTER FAILING TO PASS THE ERROR
C                            TEST EVEN AFTER REDUCING H BY A FACTOR
C                            OF 1.0E10 FROM ITS INITIAL VALUE.
C                            SEE REMARKS.
C                          IER = 133, IMPLIES THE INTEGRATION WAS
C                            HALTED AFTER FAILING TO ACHIEVE
C                            CORRECTOR CONVERGENCE EVEN AFTER
C                            REDUCING H BY A FACTOR OF 1.0E10 FROM
C                            ITS INITIAL VALUE. SEE REMARKS.
C                          IER = 134, IMPLIES THAT AFTER SOME INITIAL
C                            SUCCESS, THE INTEGRATION WAS HALTED EITHER
C                            BY REPEATED ERROR TEST FAILURES OR BY
C                            A TEST ON TOL. SEE REMARKS.
C                          IER = 135, IMPLIES THAT ONE OF THE INPUT
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C                                PARAMETERS N,X,H,XEND,TOL,METH,MITER, OR
C                                INDEX WAS SPECIFIED INCORRECTLY.
C                              IER = 136, IMPLIES THAT INDEX HAD A VALUE
C                                OF -1 ON INPUT, BUT THE DESIRED CHANGES
C                                OF PARAMETERS WERE NOT IMPLEMENTED
C                                BECAUSE XEND WAS NOT BEYOND X.
C                                INTERPOLATION TO X = XEND WAS PERFORMED.
C                                TO TRY AGAIN, SIMPLY CALL AGAIN WITH
C                                INDEX EQUAL TO -1 AND A NEW VALUE FOR
C                                XEND.
C
C    PRECISION/HARDWARE   - SINGLE AND DOUBLE/H32
C                         - SINGLE/H36,H48,H60
C
C    REQD. IMSL ROUTINES - DGRCS,DGRIN,DGRPS,DGRST,LUDATF,LUELMF,UERTST,
C                            UGETIO
C
C    NOTATION            - INFORMATION ON SPECIAL NOTATION AND
C                            CONVENTIONS IS AVAILABLE IN THE MANUAL
C                            INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
C
C    REMARKS  1.  THE EXTERNAL SUBROUTINE FCNJ IS USED ONLY WHEN
C                 INPUT PARAMETER MITER IS EQUAL TO 1. OTHERWISE, A
C                 DUMMY FUNCTION CAN BE USED. THE DUMMY SUBROUTINE
C                 SHOULD BE OF THE FOLLOWING FORM
C                   SUBROUTINE FCNJ (N,X,Y,PD)
C                   INTEGER N
C                   REAL Y(N),PD(N,N),X
C                   RETURN
C                   END
C             2.  AFTER THE INITIAL CALL, IF A NORMAL RETURN OCCURRED
C                 (IER=0) AND A NORMAL CONTINUATION IS DESIRED, SIMPLY
C                 RESET XEND AND CALL DGEAR AGAIN. ALL OTHER
C                 PARAMETERS WILL BE READY FOR THE NEXT CALL. A CHANGE
C                 OF PARAMETERS WITH INDEX EQUAL TO -1 CAN BE MADE
C                 AFTER EITHER A SUCCESSFUL OR AN UNSUCCESSFUL RETURN.
C             3.  THE COMMON BLOCK /GEAR/ USED IN DGEAR NEEDS TO BE
C                 PRESERVED BETWEEN CALLS TO DGEAR. IF IT IS NECESSARY
C                 FOR THE COMMON BLOCK TO EXIST IN THE CALLING PROGRAM
C                 THE FOLLOWING STATEMENT SHOULD BE INCLUDED
C                   COMMON  /GEAR/ DUMMY(48),SDUMMY(4),IDUMMY(38)
C                 WHERE DUMMY, SDUMMY, AND IDUMMY ARE VARIABLE NAMES NOT
C                 USED ELSEWHERE IN THE CALLING PROGRAM.  (FOR DOUBLE
C                 PRECISION DUMMY IS TYPE DOUBLE AND SDUMMY IS TYPE REAL)
C             4.  THE CHOICE OF VALUES FOR METH AND MITER MAY REQUIRE
C                 SOME EXPERIMENTATION, AND ALSO SOME CONSIDERATION OF
C                 THE NATURE OF THE PROBLEM AND OF STORAGE REQUIREMENTS.
C                 THE PRIME CONSIDERATION IS STIFFNESS. IF
C                 THE PROBLEM IS NOT STIFF, THE BEST CHOICE IS PROBABLY
C                 METH = 1 WITH MITER = 0. IF THE PROBLEM IS STIFF TO A
C                 SIGNIFICANT DEGREE, THEN METH SHOULD BE 2 AND MITER
C                 SHOULD BE 1, 2, OR 3. IF THE USER HAS NO KNOWLEDGE OF
C                 THE INHERENT TIME CONSTANTS OF THE PROBLEM, WITH
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C     WHICH TO PREDICT ITS STIFFNESS, ONE WAY TO DETERMINE
C     THIS IS TO TRY METH = 1 AND MITER = 0 FIRST, AND LOOK
C     AT THE BEHAVIOR OF THE SOLUTION COMPUTED AND THE STEP
C     SIZES USED. IF THE TYPICAL VALUES OF H ARE MUCH
C     SMALLER THAN THE SOLUTION BEHAVIOR WOULD SEEM TO
C     REQUIRE (THAT IS, MORE THAN 100 STEPS ARE TAKEN OVER
C     AN INTERVAL IN WHICH THE SOLUTIONS CHANGE BY LESS
C     THAN ONE PERCENT), THEN THE PROBLEM IS PROBABLY STIFF
C     AND THE DEGREE OF STIFFNESS CAN BE ESTIMATED FROM THE
C     VALUES OF H USED AND THE SMOOTHNESS OF THE SOLUTION.
C     IF THE DEGREE OF STIFFNESS IS ONLY SLIGHT, IT MAY BE
C     THAT METH = 1 IS MORE EFFICIENT THAN METH = 2.
C     EXPERIMENTATION WOULD BE REQUIRED TO DETERMINE THIS.
C     REGARDLESS OF METH, THE LEAST EFFECTIVE VALUE OF
C     MITER IS 0, AND THE MOST EFFECTIVE IS 1 OR 2.
C     MITER = 3 IS GENERALLY SOMEWHERE IN BETWEEN. SINCE
C     THE STORAGE REQUIREMENTS GO UP IN THE SAME ORDER AS
C     EFFECTIVENESS, TRADE-OFF CONSIDERATIONS ARE
C     NECESSARY. FOR REASONS OF ACCURACY AND SPEED, THE
C     CHOICE OF MITER = 1 IS GENERALLY PREFERRED TO
C     MITER = 2, UNLESS THE SYSTEM IS FAIRLY COMPLICATED
C     (AND FCNJ IS THUS NOT FEASIBLE TO CODE). THE
C     ACCURACY OF THE FCNJ CALCULATION CAN BE CHECKED BY
C     COMPARISON OF THE JACOBIAN WITH THAT GENERATED WITH
C     MITER = 2. IF THE JACOBIAN MATRIX IS SIGNIFICANTLY
C     DIAGONALLY DOMINANT, THEN THE OPTION MITER = 3 IS
C     LIKELY TO BE NEARLY AS EFFECTIVE AS MITER = 1 OR 2,
C     AND WILL SAVE CONSIDERABLE STORAGE AND RUN TIME.
C     IT IS POSSIBLE, AND POTENTIALLY QUITE DESIRABLE, TO
C     USE DIFFERENT VALUES OF METH AND MITER IN DIFFERENT
C     SUBINTERVALS OF THE PROBLEM. FOR EXAMPLE, IF THE
C     PROBLEM IS NON-STIFF INITIALLY AND STIFF LATER,
C     METH = 1 AND MITER = 0 MIGHT BE SET INITIALLY, AND
C     METH = 2 AND MITER = 1 LATER.
C  5. THE INITIAL VALUE OF THE STEP SIZE, H, SHOULD BE
C     CHOSEN CONSIDERABLY SMALLER THAN THE AVERAGE VALUE
C     EXPECTED FOR THE PROBLEM, AS THE FIRST-ORDER METHOD
C     WITH WHICH DGEAR BEGINS IS NOT GENERALLY THE MOST
C     EFFICIENT ONE. HOWEVER, FOR THE FIRST STEP, AS FOR
C     EVERY STEP, DGEAR TESTS FOR THE POSSIBILITY THAT
C     THE STEP SIZE WAS TOO LARGE TO PASS THE ERROR TEST
C     (BASED ON TOL), AND IF SO ADJUSTS THE STEP SIZE
C     DOWN AUTOMATICALLY. THIS DOWNWARD ADJUSTMENT, IF
C     ANY, IS NOTED BY IER HAVING THE VALUES 66 OR 67,
C     AND SUBSEQUENT RUNS ON THE SAME OR SIMILAR PROBLEM
C     SHOULD BE STARTED WITH AN APPROPRIATELY SMALLER
C     VALUE OF H.
C  6. SOME OF THE VALUES OF INTEREST LOCATED IN THE
C     COMMON BLOCK /GEAR/ ARE
C     A. HUSED, THE STEP SIZE H LAST USED SUCCESSFULLY
C        (DUMMY(8))
C     B. NQUSED, THE ORDER LAST USED SUCCESSFULLY
C        (IDUMMY(6))
C
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C               C. NSTEP, THE CUMULATIVE NUMBER OF STEPS TAKEN
C                  (IDUMMY(7))
C               D. NFE, THE CUMULATIVE NUMBER OF FCN EVALUATIONS
C                  (IDUMMY(8))
C               E. NJE, THE CUMULATIVE NUMBER OF JACOBIAN
C                  EVALUATIONS, AND HENCE ALSE OF MATRIX LU
C                  DECOMPOSITIONS (IDUMMY(9))
C            7. THE NORMAL USAGE OF DGEAR MAY BE SUMMARIZED AS FOLLOWS
C               A. SET THE INITIAL VALUES IN Y.
C               B. SET N, X, H, TOL, METH, AND MITER.
C               C. SET XEND TO THE FIRST OUTPUT POINT, AND INDEX TO 1.
C               D. CALL DGEAR
C               E. EXIT IF IER IS GREATER THAN 128.
C               F. OTHERWISE, DO DESIRED OUTPUT OF Y.
C               G. EXIT IF THE PROBLEM IS FINISHED.
C               H. OTHERWISE, RESET XEND TO THE NEXT OUTPUT POINT, AND
C                  RETURN TO STEP D.
C            8. THE ERROR WHICH IS CONTROLLED BY WAY OF THE PARAMETER
C               TOL IS AN ESTIMATE OF THE LOCAL TRUNCATION ERROR, THAT
C               IS, THE ERROR COMMITTED ON TAKING A SINGLE STEP WITH
C               THE METHOD, STARTING WITH DATA REGARDED AS EXACT. THIS
C               IS TO BE DISTINGUISHED FROM THE GLOBAL TRUNCATION
C               ERROR, WHICH IS THE ERROR IN ANY GIVEN COMPUTED VALUE
C               OF Y(X) AS A RESULT OF THE LOCAL TRUNCATION ERRORS
C               FROM ALL STEPS TAKEN TO OBTAIN Y(X). THE LATTER ERROR
C               ACCUMULATES IN A NON-TRIVIAL WAY FROM THE LOCAL
C               ERRORS, AND IS NEITHER ESTIMATED NOR CONTROLLED BY
C               THE ROUTINE. SINCE IT IS USUALLY THE GLOBAL ERROR THAT
C               A USER WANTS TO HAVE UNDER CONTROL, SOME
C               EXPERIMENTATION MAY BE NECESSARY TO GET THE RIGHT
C               VALUE OF TOL TO ACHIEVE THE USERS NEEDS. IF THE
C               PROBLEM IS MATHEMATICALLY STABLE, AND THE METHOD USED
C               IS APPROPRIATELY STABLE, THEN THE GLOBAL ERROR AT A
C               GIVEN X SHOULD VARY SMOOTHLY WITH TOL IN A MONOTONE
C               INCREASING MANNER.
C            9. IF THE ROUTINE RETURNS WITH IER VALUES OF 132, 133,
C               OR 134, THE USER SHOULD CHECK TO SEE IF TOO MUCH
C               ACCURACY IS BEING REQUIRED. THE USER MAY WISH TO
C               SET TOL TO A LARGER VALUE AND CONTINUE. ANOTHER
C               POSSIBLE CAUSE OF THESE ERROR CONDITIONS IS AN
C               ERROR IN THE CODING OF THE EXTERNAL FUNCTIONS FCN
C               OR FCNJ. IF NO ERRORS ARE FOUND, IT MAY BE NECESSARY
C               TO MONITOR INTERMEDIATE QUANTITIES GENERATED BY THE
C               ROUTINE. THESE QUANTITIES ARE STORED IN THE WORK VECTOR
C               WK AND INDEXED BY SPECIFIC ELEMENTS IN THE COMMON BLOCK
C               /GEAR/. IF IER IS 132 OR 134, THE COMPONENTS CAUSING
C               THE ERROR TEST FAILURE CAN BE IDENTIFIED FROM LARGE
C               VALUES OF THE QUANTITY
C                 WK(IDUMMY(11)+I)/WK(I), FOR I=1,...,N.
C               ONE CAUSE OF THIS MAY BE A VERY SMALL BUT NONZERO
C               INITIAL VALUE OF ABS(Y(I)).
C               IF IER IS 133, SEVERAL POSSIBILITIES EXIST.
C               IT MAY BE INSTRUCTIVE TO TRY DIFFERENT VALUES OF MITER.
```

```
C                ALTERNATIVELY, THE USER MIGHT MONITOR SUCCESSIVE
C                CORRECTOR ITERATES CONTAINED IN WK(IDUMMY(12)+I), FOR
C                I=1,...,N. ANOTHER POSSIBILITY MIGHT BE TO MONITOR
C                THE JACOBIAN MATRIX, IF ONE IS USED, STORED, BY
C                COLUMN, IN WK(IDUMMY(10)+I), FOR I=1,...,N*N IF
C                MITER IS EQUAL TO 1 OR 2, OR FOR I=1,...,N IF
C                MITER IS EQUAL TO 3.
C
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C
C   WARRANTY             - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN
C                          APPLIED TO THIS CODE. NO OTHER WARRANTY,
C                          EXPRESSED OR IMPLIED, IS APPLICABLE.
C
C-----------------------------------------------------------------------
      SUBROUTINE DGEAR  (N,FCN,FCNJ,X,H,Y,XEND,TOL,METH,MITER,INDEX,
     1                   IWK,WK,IER)
C-----------------------------------------------------------------------
      INTEGER        N,METH,MITER,INDEX,IWK(1),IER
      REAL           X,H,Y(N),XEND,TOL,WK(1)
C                           SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER        NERROR,NSAVE1,NSAVE2,NPW,NY,NC,MFC,KFLAG,
     1               JSTART,NSQ,NQUSED,NSTEP,NFE,NJE,I,NO,NHCUT,KGO,
     2               JER,KER,NN,NEQUIL,IDUMMY(21)
      REAL           SDUMMY(4),KEFF
      REAL           T,HH,HMIN,HMAX,EPSC,UROUND,EPSJ,HUSED,TOUTP,
     1               AYI,D,DN,SEPS,DUMMY(39)
      EXTERNAL       FCN,FCNJ
      COMMON /GEAR/ T,HH,HMIN,HMAX,EPSC,UROUND,EPSJ,HUSED,DUMMY,
     1               TOUTP,SDUMMY,NC,MFC,KFLAG,JSTART,NSQ,NQUSED,
     2               NSTEP,NFE,NJE,NPW,NERROR,NSAVE1,NSAVE2,NEQUIL,
     3               NY,IDUMMY,NO,NHCUT
      COMMON/LOCAL /IZ,ICOUNT,IFLAGA,JL,JJ,HW,HWO,R(6),RH2,RCO,
     1              DELH(7),DELH2,DELCO,DELTAZ,RECORE,DENSB,DENSP,
     2              FSTAR,TCORS,TCOR,TANN,GIBB(7),H2OSAT,
     3              KEFF,OPPOSE(9),GASFLO
      DATA           SEPS/0.145519152284E-11/
C-----------------------------------------------------------------------
      KER = 0
      JER = 0
      UROUND = SEPS
C                                     COMPUTE WORK VECTOR INDICIES
      NERROR = N
      NSAVE1 = NERROR+N
      NSAVE2 = NSAVE1+N
      NPW = NSAVE2+N
      NEQUIL = NPW
      IF (MITER.EQ.1.OR.MITER.EQ.2) NEQUIL = NPW+N*N
      IF (MITER.EQ.1.OR.MITER.EQ.2) NY = NPW+N*N+N
      IF (MITER.EQ.3) NY = NPW+N
      IF (MITER.EQ.0) NY = NPW+1
      MFC = 10*METH+MITER
C                                     CHECK FOR INCORRECT INPUT PARAMETERS
```

```
C
      IF (MITER.LT.0.OR.MITER.GT.3) GO TO 85
      IF (METH.NE.1.AND.METH.NE.2) GO TO 85
      IF (TOL.LE.0.) GO TO 85
      IF (N.LE.0) GO TO 85
      IF ((X-XEND)*H.GE.0.) GO TO 85
      IF (INDEX.EQ.0) GO TO 10
      IF (INDEX.EQ.2) GO TO 15
      IF (INDEX.EQ.-1) GO TO 20
      IF (INDEX.EQ.3) GO TO 25
      IF (INDEX.NE.1) GO TO 85
C                                     IF INITIAL VALUES OF YMAX OTHER THAN
C                                       THOSE SET BELOW ARE DESIRED, THEY
C                                       SHOULD BE SET HERE. ALL YMAX(I)
C                                       MUST BE POSITIVE. IF VALUES FOR
C                                       HMIN OR HMAX, THE BOUNDS ON
C                                       DABS(HH), OTHER THAN THOSE BELOW
C                                       ARE DESIRED, THEY SHOULD BE SET
C                                       BELOW.
      DO 5 I=1,N
         WK(I) = ABS(Y(I))
         IF (WK(I).EQ.0.) WK(I) = 1.
         WK(NY+I) = Y(I)
    5 CONTINUE
      NC = N
      T = X
      HH = H
      IF ((T+HH).EQ.T) KER = 33
      HMIN = ABS(H)
      HMAX = ABS(X-XEND)*10.
      EPSC = TOL
      JSTART = 0
      NO = N
      NSQ = NO*NO
      EPSJ = SQRT(UROUND)
      NHCUT = 0
      DUMMY(2) = 1.0
      DUMMY(14) = 1.0
      GO TO 30
C                                     TOUTP IS THE PREVIOUS VALUE OF XEND
C                                       FOR USE IN HMAX.
   10 HMAX = ABS(XEND-TOUTP)*10.
      GO TO 45
C
   15 HMAX = ABS(XEND-TOUTP)*10.
      IF ((T-XEND)*HH.GE.0.) GO TO 95
      GO TO 50
C
   20 IF ((T-XEND)*HH.GE.0.) GO TO 90
      JSTART = -1
      NC = N
      EPSC = TOL
C
```

```
   25 IF ((T+HH).EQ.T) KER = 33
C
   30 NN = NO
      CALL DGRST (FCN,FCNJ,WK(NY+1),WK,WK(NERROR+1),WK(NSAVE1+1),
     1 WK(NSAVE2+1),WK(NPW+1),WK(NEQUIL+1),IWK,NN)
C
      KGO = 1-KFLAG
      GO TO (35,55,70,80), KGO
C                                     KFLAG = 0, -1, -2, -3
   35 CONTINUE
C                                     NORMAL RETURN FROM INTEGRATOR. THE
C                                       WEIGHTS YMAX(I) ARE UPDATED. IF
C                                       DIFFERENT VALUES ARE DESIRED, THEY
C                                       SHOULD BE SET HERE. A TEST IS MADE
C                                       FOR TOL BEING TOO SMALL FOR THE
C                                       MACHINE PRECISION. ANY OTHER TESTS
C                                       OR CALCULATIONS THAT ARE REQUIRED
C                                       AFTER EVERY STEP SHOULD BE
C                                       INSERTED HERE. IF INDEX = 3, Y IS
C                                       SET TO THE CURRENT SOLUTION ON
C                                       RETURN. IF INDEX = 2, HH IS
C                                       CONTROLLED TO HIT XEND (WITHIN
C                                       ROUNDOFF ERROR), AND THEN THE
C                                       CURRENT SOLUTION IS PUT IN Y ON
C                                       RETURN. FOR ANY OTHER VALUE OF
C                                       INDEX, CONTROL RETURNS TO THE
C                                       INTEGRATOR UNLESS XEND HAS BEEN
C                                       REACHED. THEN INTERPOLATED VALUES
C                                       OF THE SOLUTION ARE COMPUTED AND
C                                       STORED IN Y ON RETURN.
C                                       IF INTERPOLATION IS NOT
C                                       DESIRED, THE CALL TO DGRIN SHOULD
C                                       BE REMOVED AND CONTROL TRANSFERRED
C                                       TO STATEMENT 95 INSTEAD OF 105.
      D = 0.
      DO 40 I=1,N
         AYI = ABS(WK(NY+I))
         WK(I) = AMAX1(WK(I),AYI)
   40 D = D+(AYI/WK(I))**2
      D = D*(UROUND/TOL)**2
      DN = N
      IF (D.GT.DN) GO TO 75
      IF (INDEX.EQ.3) GO TO 95
      IF (INDEX.EQ.2) GO TO 50
   45 IF ((T-XEND)*HH.LT.0.) GO TO 25
      NN = NO
      CALL DGRIN (XEND,WK(NY+1),NN,Y)
      X = XEND
      GO TO 105
   50 IF (((T+HH)-XEND)*HH.LE.0.) GO TO 25
      IF (ABS(T-XEND).LE.100.*UROUND*HMAX) GO TO 95
      IF ((T-XEND)*HH.GE.0.) GO TO 95
      HH = (XEND-T)*(1.-4.*UROUND)
```

```
      JSTART = -1
      GO TO 25
C                                        ON AN ERROR RETURN FROM INTEGRATOR,
C                                          AN IMMEDIATE RETURN OCCURS IF
C                                          KFLAG = -2, AND RECOVERY ATTEMPTS
C                                          ARE MADE OTHERWISE. TO RECOVER, HH
C                                          AND HMIN ARE REDUCED BY A FACTOR
C                                          OF .1 UP TO 10 TIMES BEFORE GIVING
C                                          UP.
   55 JER = 66
   60 IF (NHCUT.EQ.10) GO TO 65
      NHCUT = NHCUT+1
      HMIN = HMIN*.1
      HH = HH*.1
      JSTART = -1
      GO TO 25
C
   65 IF (JER.EQ.66) JER = 132
      IF (JER.EQ.67) JER = 133
      GO TO 95
C
   70 JER = 134
      GO TO 95
C
   75 JER = 134
      KFLAG = -2
      GO TO 95
C
   80 JER = 67
      GO TO 60
C
   85 JER = 135
      GO TO 110
C
   90 JER = 136
      NN = NO
      CALL DGRIN (XEND,WK(NY+1),NN,Y)
      X = XEND
      GO TO 110
C
   95 X = T
      DO 100 I=1,N
  100 Y(I) = WK(NY+I)
  105 IF (JER.LT.128) INDEX = KFLAG
      TOUTP = X
      H = HUSED
      IF (KFLAG.NE.0) H = HH
  110 IER = MAXO(KER,JER)
 9000 CONTINUE
      IF (KER.NE.0.AND.JER.LT.128) CALL UERTST (KER,6HDGEAR )
      IF (JER.NE.0) CALL UERTST (JER,6HDGEAR )
 9005 RETURN
      END
```

```
C   IMSL ROUTINE NAME   - DGRCS
C
C-----------------------------------------------------------------------
C
C   COMPUTER            - BGH/SINGLE
C
C   LATEST REVISION     - JANUARY 1, 1978
C
C   PURPOSE             - NUCLEUS CALLED ONLY BY IMSL SUBROUTINE DGEAR
C
C   PRECISION/HARDWARE  - SINGLE AND DOUBLE/H32
C                       - SINGLE/H36,H48,H60
C
C   REQD. IMSL ROUTINES - NONE REQUIRED
C
C   NOTATION            - INFORMATION ON SPECIAL NOTATION AND
C                         CONVENTIONS IS AVAILABLE IN THE MANUAL
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C                         EXPRESSED OR IMPLIED, IS APPLICABLE.
C
C-----------------------------------------------------------------------
      SUBROUTINE DGRCS  (METH,NQ,EL,TQ,MAXDER)
C-----------------------------------------------------------------------
      INTEGER             METH,NQ,MAXDER
      REAL                TQ(1)
      REAL                EL(1)
                                SPECIFICATIONS FOR LOCAL VARIABLES
C
      INTEGER             K
      REAL                PERTST(12,2,3)
      DATA                PERTST/1.,1.,2.,1.,.3158,.7407E-1,
     1                    .1391E-1,.2182E-2,.2945E-3,.3492E-4,
     2                    .3692E-5,.3524E-6,1.,1.,.5,.1667,
     3                    .4167E-1,7*1.,2.,12.,24.,37.89,
     4                    53.33,70.08,87.97,106.9,126.7,
     5                    147.4,168.8,191.0,2.0,4.5,7.333,
     6                    10.42,13.7,7*1.,12.0,24.0,37.89,
     7                    53.33,70.08,87.97,106.9,126.7,
     8                    147.4,168.8,191.0,1.,3.0,6.0,
     9                    9.167,12.5,8*1./
C-----------------------------------------------------------------------
      GO TO (5,10), METH
    5 MAXDER = 12
      GO TO (15,20,25,30,35,40,45,50,55,60,65,70), NQ
   10 MAXDER = 5
      GO TO (75,80,85,90,95), NQ
                                THE FOLLOWING COEFFICIENTS SHOULD BE
C                                 DEFINED TO MACHINE ACCURACY. FOR A
C
```

```
C                                       GIVEN ORDER NQ, THEY CAN BE
C                                       CALCULATED BY USE OF THE
C                                       GENERATING POLYNOMIAL L(T), WHOSE
C                                       COEFFICIENTS ARE EL(I).. L(T) =
C                                       EL(1) + EL(2)*T + ... +
C                                       EL(NQ+1)*T**NQ. FOR THE IMPLICIT
C                                       ADAMS METHODS, L(T) IS GIVEN BY
C                                       DL/DT = (T+1)*(T+2)* ...
C                                       *(T+NQ-1)/K, L(-1) = 0, WHERE K =
C                                       FACTORIAL(NQ-1). FOR THE GEAR
C                                       METHODS, L(T) = (T+1)*(T+2)* ...
C                                       *(T+NQ)/K, WHERE K =
C                                       FACTORIAL(NQ)*(1 + 1/2 + ... +
C                                       1/NQ). THE ORDER IN WHICH THE
C                                       GROUPS APPEAR BELOW IS.. IMPLICIT
C                                       ADAMS METHODS OF ORDERS 1 TO 12,
C                                       BACKWARD DIFFERENTIATION METHODS
C                                       OF ORDERS 1 TO 5.
   15 EL(1) = 1.0
      GO TO 100
   20 EL(1) = 0.5
      EL(3) = 0.5
      GO TO 100
   25 EL(1) = 4.1666666667E-01
      EL(3) = 0.75
      EL(4) = 1.6666666667E-01
      GO TO 100
   30 EL(1) = 0.375
      EL(3) = 9.1666666667E-01
      EL(4) = 3.3333333333E-01
      EL(5) = 4.1666666667E-02
      GO TO 100
   35 EL(1) = 3.4861111111E-01
      EL(3) = 1.0416666667E0
      EL(4) = 4.8611111111E-01
      EL(5) = 1.0416666667E-01
      EL(6) = 8.3333333333E-03
      GO TO 100
   40 EL(1) = 3.2986111111E-01
      EL(3) = 1.1416666667E+00
      EL(4) = 0.625E+00
      EL(5) = 1.7708333333E-01
      EL(6) = 0.025E+00
      EL(7) = 1.3888888889E-03
      GO TO 100
   45 EL(1) = 3.1559193122E-01
      EL(3) = 1.225E+00
      EL(4) = 7.5185185185E-01
      EL(5) = 2.5520833333E-01
      EL(6) = 4.8611111111E-02
      EL(7) = 4.8611111111E-03
      EL(8) = 1.9841269841E-04
      GO TO 100
```

```
50 EL(1) = 3.0422453704E-01
   EL(3) = 1.2964285714E+00
   EL(4) = 8.6851851852E-01
   EL(5) = 3.3576388889E-01
   EL(6) = 7.7777777778E-02
   EL(7) = 1.0648148148E-02
   EL(8) = 7.9365079365E-04
   EL(9) = 2.4801587302E-05
   GO TO 100
55 EL(1) = 2.9486800044E-01
   EL(3) = 1.3589285714E+00
   EL(4) = 9.7655423280E-01
   EL(5) = 4.171875E-01
   EL(6) = 1.1135416667E-01
   EL(7) = 0.01875E+00
   EL(8) = 1.9345238095E-03
   EL(9) = 1.1160714286E-04
   EL(10)= 2.7557319224E-06
   GO TO 100
60 EL(1) = 2.8697544643E-01
   EL(3) = 1.4144841270E+00
   EL(4) = 1.0772156085E+00
   EL(5) = 4.9856701940E-01
   EL(6) = 1.484375E-01
   EL(7) = 2.9060570988E-02
   EL(8) = 3.7202380952E-03
   EL(9) = 2.9968584656E-04
   EL(10)= 1.3778659612E-05
   EL(11)= 2.7557319224E-07
   GO TO 100
65 EL(1) = 2.8018959644E-01
   EL(3) = 1.4644841270E+00
   EL(4) = 1.1715145503E+00
   EL(5) = 5.7935819004E-01
   EL(6) = 1.8832286155E-01
   EL(7) = 4.1430362654E-02
   EL(8) = 6.2111441799E-03
   EL(9) = 6.2520667989E-04
   EL(10)= 4.0417401529E-05
   EL(11)= 1.5156525573E-06
   EL(12)= 2.5052108385E-08
   GO TO 100
70 EL(1) = 2.7426554003E-01
   EL(3) = 1.5099386724E+00
   EL(4) = 1.2602711640E+00
   EL(5) = 6.5923418210E-01
   EL(6) = 2.3045800265E-01
   EL(7) = 5.5697246105E-02
   EL(8) = 9.4394841270E-03
   EL(9) = 1.1192749669E-03
   EL(10) = 9.0939153439E-05
   EL(11) = 4.8225308642E-06
   EL(12)= 1.5031265031E-07
```

```
      EL(13)= 2.0876756988E-09
      GO TO 100
C
   75 EL(1) = 1.0E+00
      GO TO 100
   80 EL(1) = 6.6666666667E-01
      EL(3) = 3.3333333333E-01
      GO TO 100
   85 EL(1) = 5.4545454545E-01
      EL(3) = EL(1)
      EL(4) = 9.0909090909E-02
      GO TO 100
   90 EL(1) = 0.48E+00
      EL(3) = 0.7E+00
      EL(4) = 0.2E+00
      EL(5) = 0.02E+00
      GO TO 100
   95 EL(1) = 4.3795620438E-01
      EL(3) = 8.2116788321E-01
      EL(4) = 3.1021897810E-01
      EL(5) = 5.4744525547E-02
      EL(6) = 3.6496350365E-03
C
  100 DO 105 K=1,3
         TQ(K) = PERTST(NQ,METH,K)
  105 CONTINUE
      TQ(4) = .5*TQ(2)/(NQ+2)
      RETURN
      END
```

```
C    IMSL ROUTINE NAME    - DGRIN
C
C-----------------------------------------------------------------------
C
C    COMPUTER             - BGH/SINGLE
C
C    LATEST REVISION      - JANUARY 1, 1978
C
C    PURPOSE              - NUCLEUS CALLED ONLY BY IMSL SUBROUTINE DGEAR
C
C    PRECISION/HARDWARE   - SINGLE AND DOUBLE/H32
C                         - SINGLE/H36,H48,H60
C
C    REQD. IMSL ROUTINES  - NONE REQUIRED
C
C    NOTATION             - INFORMATION ON SPECIAL NOTATION AND
C                             CONVENTIONS IS AVAILABLE IN THE MANUAL
C                             INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
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C
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C                             APPLIED TO THIS CODE. NO OTHER WARRANTY,
C                             EXPRESSED OR IMPLIED, IS APPLICABLE.
C
C
C=======================================================================
      SUBROUTINE DGRIN  (TOUT,Y,NO,YO)
C=======================================================================
      INTEGER             NO
      REAL                TOUT,YO(NO),Y(NO,1)
C                                 SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER             NC,MFC,KFLAG,I,L,J,JSTART,NSQ,NQUSED,NSTEP,
     1                    NFE,NJE,NPW,NERROR,NSAVE1,NSAVE2,NEQUIL,NY,
     2                    IDUMMY(23)
      REAL                SDUMMY(4)
      REAL                T,H,HMIN,HMAX,EPSC,UROUND,EPSJ,HUSED,S,S1,
     1                    DUMMY(40)
      COMMON /GEAR/       T,H,HMIN,HMAX,EPSC,UROUND,EPSJ,HUSED,DUMMY,
     1                    SDUMMY,NC,MFC,KFLAG,JSTART,NSQ,NQUSED,NSTEP,
     2                    NFE,NJE,NPW,NERROR,NSAVE1,NSAVE2,NEQUIL,NY,
     3                    IDUMMY
C-----------------------------------------------------------------------
      DO 5 I = 1,NC
         YO(I) = Y(I,1)
    5 CONTINUE
C                                     THIS SUBROUTINE COMPUTES INTERPOLATED
C                                       VALUES OF THE DEPENDENT VARIABLE
C                                       Y AND STORES THEM IN YO. THE
C                                       INTERPOLATION IS TO THE
C                                       POINT T = TOUT, AND USES THE
C                                       NORDSIECK HISTORY ARRAY Y, AS
C                                       FOLLOWS..
```

```
C                                                    NQ
C                                    YO(I)    =     SUM   Y(I,J+1)*S**J ,
C                                                    J=0
C                                    WHERE S  =  -(T-TOUT)/H.
      L = JSTART + 1
      S = (TOUT - T)/H
      S1 = 1.0
      DO 15 J = 2,L
         S1 = S1*S
         DO 10 I = 1,NC
            YO(I) = YO(I) + S1*Y(I,J)
   10    CONTINUE
   15 CONTINUE
      RETURN
      END
```

```
C   IMSL ROUTINE NAME   - DGRPS
C
C-----------------------------------------------------------------------
C
C   COMPUTER            - BGH/SINGLE
C
C   LATEST REVISION     - JANUARY 1, 1978
C
C   PURPOSE             - NUCLEUS CALLED ONLY BY IMSL SUBROUTINE DGEAR
C
C   PRECISION/HARDWARE  - SINGLE AND DOUBLE/H32
C                       - SINGLE/H36,H48,H60
C
C   REQD. IMSL ROUTINES - LUDATF,UERTST,UGETIO
C
C   NOTATION            - INFORMATION ON SPECIAL NOTATION AND
C                           CONVENTIONS IS AVAILABLE IN THE MANUAL
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C                           EXPRESSED OR IMPLIED, IS APPLICABLE.
C
C
C=======================================================================
      SUBROUTINE DGRPS  (FCN,FCNJ,Y,NO,CON,MITER,YMAX,SAVE1,SAVE2,PW,
     1                   EQUIL,IPIV,IER)
C=======================================================================
      INTEGER           NO,MITER,IPIV(1),IER
      REAL              Y(NO,1),CON,YMAX(1),SAVE1(1),SAVE2(1),PW(1),
     1                  EQUIL(1)
C                                 SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER           NC,MFC,KFLAG,JSTART,NQUSED,NSTEP,NFE,NJE,NPW,
     1                  NSQ,I,J1,J,NERROR,NSAVE1,NSAVE2,NEQUIL,NY,
     2                  IDUMMY(23)
      REAL              SDUMMY(4)
      REAL              T,H,HMIN,HMAX,EPSC,UROUND,EPSJ,HUSED,D,RO,YJ,R,
     1                  D1,D2,WA,DUMMY(40)
      EXTERNAL          FCN,FCNJ
      COMMON /GEAR/     T,H,HMIN,HMAX,EPSC,UROUND,EPSJ,HUSED,DUMMY,
     1                  SDUMMY,NC,MFC,KFLAG,JSTART,NSQ,NQUSED,NSTEP,
     2                  NFE,NJE,NPW,NERROR,NSAVE1,NSAVE2,NEQUIL,NY,
     3                  IDUMMY
C-----------------------------------------------------------------------
      IF (MITER .EQ. 2) GO TO 10
C                                 THIS ROUTINE IS CALLED BY DGRST TO
C                                   COMPUTE AND PROCESS THE MATRIX
C                                   P = I - H*EL(1)*J , WHERE J IS AN
C                                   APPROXIMATION TO THE JACOBIAN.
C                                   J IS COMPUTED, EITHER BY THE USER-
C                                   SUPPLIED ROUTINE FCNJ
```

```
C                                       IF MITER = 1, OR BY FINITE
C                                       DIFFERENCING IF MITER = 2.
C                                       J IS STORED IN PW AND REPLACED BY
C                                       P, USING CON = -H*EL(1).
C                                       THEN P IS SUBJECTED TO LU
C                                       DECOMPOSITION IN PREPARATION FOR
C                                       LATER SOLUTION OF LINEAR SYSTEMS
C                                       WITH P AS COEFFICIENT MATRIX.
C                                       IN ADDITION TO VARIABLES DESCRIBED
C                                       PREVIOUSLY, COMMUNICATION
C                                       WITH DGRPS USES THE FOLLOWING
C                                       EPSJ = DSQRT(UROUND), USED IN THE
C                                       NUMERICAL JACOBIAN INCREMENTS.
C                                       NSQ = NO**2.
C                                       IF MITER = 1, CALL FCNJ AND
C                                       MULTIPLY BY SCALAR.
      CALL FCNJ (NC,T,Y,PW)
      DO 5 I = 1,NSQ
    5    PW(I) = PW(I)*CON
      GO TO 30
C                                     IF MITER = 2, MAKE NC CALLS TO FCN TO
C                                       APPROXIMATE J.
   10 D = 0.0
      DO 15 I = 1,NC
   15    D = D + SAVE2(I)**2
      RO = ABS(H)*SQRT(D)*1.0E+03*UROUND
      J1 = 0
      DO 25 J = 1,NC
         YJ = Y(J,1)
         R = EPSJ*YMAX(J)
         R = AMAX1(R,RO)
         Y(J,1) = Y(J,1) + R
         D = CON/R
         CALL FCN (NC,T,Y,SAVE1)
         DO 20 I = 1,NC
   20       PW(I+J1) = (SAVE1(I) - SAVE2(I))*D
         Y(J,1) = YJ
         J1 = J1 + NO
   25 CONTINUE
C                                     ADD IDENTITY MATRIX.
   30 J = 1
      DO 35 I = 1,NC
         PW(J) = PW(J) + 1.0
         J = J + (NO + 1)
   35 CONTINUE
C                                     DO LU DECOMPOSITION ON P.
      CALL LUDATF (PW,PW,NC,NO,0,D1,D2,IPIV,EQUIL,WA,IER)
      RETURN
      END
```

```
C    IMSL ROUTINE NAME   - DGRST
C
C-----------------------------------------------------------------------
C
C    COMPUTER            - BGH/SINGLE
C
C    LATEST REVISION     - JUNE 1, 1980
C
C    PURPOSE             - NUCLEUS CALLED ONLY BY IMSL SUBROUTINE DGEAR
C
C    PRECISION/HARDWARE  - SINGLE AND DOUBLE/H32
C                        - SINGLE/H36,H48,H60
C
C    REQD. IMSL ROUTINES - DGRCS,DGRPS,LUDATF,LUELMF,UERTST,UGETIO
C
C    NOTATION            - INFORMATION ON SPECIAL NOTATION AND
C                            CONVENTIONS IS AVAILABLE IN THE MANUAL
C                            INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
C
C    COPYRIGHT           - 1978 BY IMSL, INC. ALL RIGHTS RESERVED.
C
C    WARRANTY            - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN
C                            APPLIED TO THIS CODE. NO OTHER WARRANTY,
C                            EXPRESSED OR IMPLIED, IS APPLICABLE.
C
C
C=======================================================================
      SUBROUTINE DGRST  (FCN,FCNJ,Y,YMAX,ERROR,SAVE1,SAVE2,PW,EQUIL,
     1                   IPIV,NO)
C=======================================================================
      INTEGER           IPIV(1),NO
      REAL              Y(NO,1),YMAX(1),ERROR(1),SAVE1(1),SAVE2(1),
     1                  PW(1),EQUIL(1)
C                                 SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER           N,MF,KFLAG,JSTART,NQUSED,NSTEP,NFE,NJE,NSQ,
     1                  I,METH,MITER,NQ,L,IDOUB,MFOLD,NOLD,IRET,MEO,
     2                  MIO,IWEVAL,MAXDER,LMAX,IREDO,J,NSTEPJ,J1,J2,
     3                  M,IER,NEWQ,NPW,NERROR,NSAVE1,NSAVE2,NEQUIL,NY,
     4                  MITER1,IDUMMY(2)
      REAL              TQ(4)
      REAL              T,H,HMIN,HMAX,EPS,UROUND,HUSED,EL(13),OLDLO,
     1                  TOLD,RMAX,RC,CRATE,EPSOLD,HOLD,FN,EDN,E,EUP,
     2                  BND,RH,R1,CON,R,HLO,RO,D,PHLO,PR3,D1,ENQ3,ENQ2,
     3                  PR2,PR1,ENQ1,EPSJ,DUMMY
      EXTERNAL          FCN,FCNJ
      COMMON /GEAR/     T,H,HMIN,HMAX,EPS,UROUND,EPSJ,HUSED,
     1                  EL,OLDLO,TOLD,RMAX,RC,CRATE,EPSOLD,HOLD,FN,
     2                  EDN,E,EUP,BND,RH,R1,R,HLO,RO,D,PHLO,PR3,D1,
     3                  ENQ3,ENQ2,PR2,PR1,ENQ1,DUMMY,TQ,
     4                  N,MF,KFLAG,JSTART,NSQ,NQUSED,NSTEP,NFE,NJE,
     5                  NPW,NERROR,NSAVE1,NSAVE2,NEQUIL,NY,
     6                  I,METH,MITER,NQ,L,IDOUB,MFOLD,NOLD,IRET,MEO,
     7                  MIO,IWEVAL,MAXDER,LMAX,IREDO,J,NSTEPJ,J1,J2,
```

```
     8                    M,NEWQ,IDUMMY
C-----------------------------------------------------------------------
      KFLAG = 0
      TOLD = T
C                                       THIS ROUTINE PERFORMS ONE STEP OF
C                                         THE INTEGRATION OF AN INITIAL
C                                         VALUE PROBLEM FOR A SYSTEM OF
C                                         ORDINARY DIFFERENTIAL EQUATIONS.
      IF (JSTART.GT.0) GO TO 50
      IF (JSTART.NE.0) GO TO 10
C                                       ON THE FIRST CALL, THE ORDER IS SET
C                                         TO 1 AND THE INITIAL YDOT IS
C                                         CALCULATED. RMAX IS THE MAXIMUM
C                                         RATIO BY WHICH H CAN BE INCREASED
C                                         IN A SINGLE STEP. IT IS INITIALLY
C                                         1.E4 TO COMPENSATE FOR THE SMALL
C                                         INITIAL H, BUT THEN IS NORMALLY
C                                         EQUAL TO 10. IF A FAILURE OCCURS
C                                         (IN CORRECTOR CONVERGENCE OR ERROR
C                                         TEST), RMAX IS SET AT 2 FOR THE
C                                         NEXT INCREASE.
      CALL FCN (N,T,Y,SAVE1)
      DO 5 I=1,N
    5 Y(I,2) = H*SAVE1(I)
      METH = MF/10
      MITER = MF-10*METH
      NQ = 1
      L = 2
      IDOUB = 3
      RMAX = 1.E4
      RC = 0.
      CRATE = 1.
      HOLD = H
      MFOLD = MF
      NSTEP = 0
      NSTEPJ = 0
      NFE = 1
      NJE = 0
      IRET = 3
      GO TO 15
C                                       IF THE CALLER HAS CHANGED METH,
C                                         DGRCS IS CALLED TO SET THE
C                                         COEFFICIENTS OF THE METHOD. IF THE
C                                         CALLER HAS CHANGED N, EPS, OR
C                                         METH, THE CONSTANTS E, EDN, EUP,
C                                         AND BND MUST BE RESET. E IS A
C                                         COMPARISON FOR ERRORS OF THE
C                                         CURRENT ORDER NQ. EUP IS TO TEST
C                                         FOR INCREASING THE ORDER, EDN FOR
```

```
C                                       DECREASING THE ORDER. BND IS USED
C                                       TO TEST FOR CONVERGENCE OF THE
C                                       CORRECTOR ITERATES. IF THE CALLER
C                                       HAS CHANGED H, Y MUST BE RESCALED.
C                                       IF H OR METH HAS BEEN CHANGED,
C                                       IDOUB IS RESET TO L + 1 TO PREVENT
C                                       FURTHER CHANGES IN H FOR THAT MANY
C                                       STEPS.
   10 IF (MF.EQ.MFOLD) GO TO 25
      MEO = METH
      MIO = MITER
      METH = MF/10
      MITER = MF-10*METH
      MFOLD = MF
      IF (MITER.NE.MIO) IWEVAL = MITER
      IF (METH.EQ.MEO) GO TO 25
      IDOUB = L+1
      IRET = 1
   15 CALL DGRCS (METH,NQ,EL,TQ,MAXDER)
      LMAX = MAXDER+1
      RC = RC*EL(1)/OLDLO
      OLDLO = EL(1)
   20 FN = N
      EDN = FN*(TQ(1)*EPS)**2
      E = FN*(TQ(2)*EPS)**2
      EUP = FN*(TQ(3)*EPS)**2
      BND = FN*(TQ(4)*EPS)**2
      EPSOLD = EPS
      NOLD = N
      GO TO (30,35,50), IRET
   25 IF ((EPS.EQ.EPSOLD).AND.(N.EQ.NOLD)) GO TO 30
      IF (N.EQ.NOLD) IWEVAL = MITER
      IRET = 1
      GO TO 20
   30 IF (H.EQ.HOLD) GO TO 50
      RH = H/HOLD
      H = HOLD
      IREDO = 3
      GO TO 40
   35 RH = AMAX1(RH,HMIN/ABS(H))
   40 RH = AMIN1(RH,HMAX/ABS(H),RMAX)
      R1 = 1.
      DO 45 J=2,L
         R1 = R1*RH
      DO 45 I=1,N
   45 Y(I,J) = Y(I,J)*R1
      H = H*RH
      RC = RC*RH
      IDOUB = L+1
      IF (IREDO.EQ.0) GO TO 285
C                                       THIS SECTION COMPUTES THE PREDICTED
C                                         VALUES BY EFFECTIVELY MULTIPLYING
C                                         THE Y ARRAY BY THE PASCAL TRIANGLE
```

```
C                                       MATRIX. RC IS THE RATIO OF NEW TO
C                                       OLD VALUES OF THE COEFFICIENT
C                                       H*EL(1). WHEN RC DIFFERS FROM 1 BY
C                                       MORE THAN 30 PERCENT, OR THE
C                                       CALLER HAS CHANGED MITER, IWEVAL
C                                       IS SET TO MITER TO FORCE THE
C                                       PARTIALS TO BE UPDATED, IF
C                                       PARTIALS ARE USED. IN ANY CASE,
C                                       THE PARTIALS ARE UPDATED AT LEAST
C                                       EVERY 20-TH STEP.
   50 IF (ABS(RC-1.).GT.0.3) IWEVAL = MITER
      IF (NSTEP.GE.NSTEPJ+20) IWEVAL = MITER
      T = T+H
      DO 55 J1=1,NQ
      DO 55 J2=J1,NQ
         J = (NQ+J1)-J2
      DO 55 I=1,N
   55 Y(I,J) = Y(I,J)+Y(I,J+1)
C                                     UP TO 3 CORRECTOR ITERATIONS ARE
C                                       TAKEN. A CONVERGENCE TEST IS MADE
C                                       ON THE R.M.S. NORM OF EACH
C                                       CORRECTION, USING BND, WHICH IS
C                                       DEPENDENT ON EPS. THE SUM OF THE
C                                       CORRECTIONS IS ACCUMULATED IN THE
C                                       VECTOR ERROR(I). THE Y ARRAY IS
C                                       NOT ALTERED IN THE CORRECTOR LOOP.
C                                       THE UPDATED Y VECTOR IS STORED
C                                       TEMPORARILY IN SAVE1.
   60 DO 65 I=1,N
   65 ERROR(I) = 0.
      M = 0
      CALL FCN (N,T,Y,SAVE2)
      NFE = NFE+1
      IF (IWEVAL.LE.0) GO TO 95
C                                     IF INDICATED, THE MATRIX P = I -
C                                       H*EL(1)*J IS REEVALUATED BEFORE
C                                       STARTING THE CORRECTOR ITERATION.
C                                       IWEVAL IS SET TO 0 AS AN INDICATOR
C                                       THAT THIS HAS BEEN DONE. IF MITER
C                                       = 1 OR 2, P IS COMPUTED AND
C                                       PROCESSED IN PSET. IF MITER = 3,
C                                       THE MATRIX USED IS P = I -
C                                       H*EL(1)*D, WHERE D IS A DIAGONAL
C                                       MATRIX.
      IWEVAL = 0
      RC = 1.
      NJE = NJE+1
      NSTEPJ = NSTEP
      GO TO (75,70,80), MITER
   70 NFE = NFE+N
   75 CON = -H*EL(1)
      MITER1 = MITER
      CALL DGRPS (FCN,FCNJ,Y,NO,CON,MITER1,YMAX,SAVE1,SAVE2,PW,EQUIL,
```

```
     1 IPIV,IER)
       IF (IER.NE.0) GO TO 155
       GO TO 125
    80 R = EL(1)*.1
       DO 85 I=1,N
    85 PW(I) = Y(I,1)+R*(H*SAVE2(I)-Y(I,2))
       CALL FCN (N,T,PW,SAVE1)
       NFE = NFE+1
       HLO = H*EL(1)
       DO 90 I=1,N
          RO = H*SAVE2(I)-Y(I,2)
          PW(I) = 1.
          D = .1*RO-H*(SAVE1(I)-SAVE2(I))
          SAVE1(I) = 0.
          IF (ABS(RO).LT.UROUND*YMAX(I)) GO TO 90
          IF (ABS(D).EQ.0.) GO TO 155
          PW(I) = .1*RO/D
          SAVE1(I) = PW(I)*RO
    90 CONTINUE
       GO TO 135
    95 IF (MITER.NE.0) GO TO (125,125,105), MITER
C
C                                    IN THE CASE OF FUNCTIONAL ITERATION,
C                                      UPDATE Y DIRECTLY FROM THE RESULT
C                                      OF THE LAST FCN CALL.
       D = 0.
       DO 100 I=1,N
          R = H*SAVE2(I)-Y(I,2)
          D = D+((R-ERROR(I))/YMAX(I))**2
          SAVE1(I) = Y(I,1)+EL(1)*R
   100 ERROR(I) = R
       GO TO 145
C                                    IN THE CASE OF THE CHORD METHOD,
C                                      COMPUTE THE CORRECTOR ERROR, F SUB
C                                      (M), AND SOLVE THE LINEAR SYSTEM
C                                      WITH THAT AS RIGHT-HAND SIDE AND P
C                                      AS COEFFICIENT MATRIX, USING THE
C                                      LU DECOMPOSITION IF MITER = 1 OR
C                                      2. IF MITER = 3, THE COEFFICIENT
C                                      H*EL(1) IN P IS UPDATED.
   105 PHLO = HLO
       HLO = H*EL(1)
       IF (HLO.EQ.PHLO) GO TO 115
       R = HLO/PHLO
       DO 110 I=1,N
          D = 1.-R*(1.-1./PW(I))
          IF (ABS(D).EQ.0.) GO TO 165
   110 PW(I) = 1./D
   115 DO 120 I=1,N
   120 SAVE1(I) = PW(I)*(H*SAVE2(I)-(Y(I,2)+ERROR(I)))
       GO TO 135
   125 DO 130 I=1,N
   130 SAVE1(I) = H*SAVE2(I)-(Y(I,2)+ERROR(I))
```

```
      CALL DUELMF (PW,SAVE1,IPIV,N,NO,SAVE1)
  135 D = 0.
      DO 140 I=1,N
         ERROR(I) = ERROR(I)+SAVE1(I)
         D = D+(SAVE1(I)/YMAX(I))**2
  140 SAVE1(I) = Y(I,1)+EL(1)*ERROR(I)
C                                     TEST FOR CONVERGENCE. IF M.GT.0, THE
C                                       SQUARE OF THE CONVERGENCE RATE
C                                       CONSTANT IS ESTIMATED AS CRATE,
C                                       AND THIS IS USED IN THE TEST.
  145 IF (M.NE.0) CRATE = AMAX1(.9*CRATE,D/D1)
      IF ((D*AMIN1(1.,2.*CRATE)).LE.BND) GO TO 170
      D1 = D
      M = M+1
      IF (M.EQ.3) GO TO 150
      CALL FCN (N,T,SAVE1,SAVE2)
      GO TO 95
C                                     THE CORRECTOR ITERATION FAILED TO
C                                       CONVERGE IN 3 TRIES. IF PARTIALS
C                                       ARE INVOLVED BUT ARE NOT UP TO
C                                       DATE, THEY ARE REEVALUATED FOR THE
C                                       NEXT TRY. OTHERWISE THE Y ARRAY IS
C                                       RETRACTED TO ITS VALUES BEFORE
C                                       PREDICTION, AND H IS REDUCED, IF
C                                       POSSIBLE. IF NOT, A NO-CONVERGENCE
C                                       EXIT IS TAKEN.
  150 NFE = NFE+2
      IF (IWEVAL.EQ.-1) GO TO 165
  155 T = TOLD
      RMAX = 2.
      DO 160 J1=1,NQ
      DO 160 J2=J1,NQ
         J = (NQ+J1)-J2
      DO 160 I=1,N
  160 Y(I,J) = Y(I,J)-Y(I,J+1)
      IF (ABS(H).LE.HMIN*1.00001) GO TO 280
      RH = .25
      IREDO = 1
      GO TO 35
  165 IWEVAL = MITER
      GO TO 60
C                                     THE CORRECTOR HAS CONVERGED. IWEVAL
C                                       IS SET TO -1 IF PARTIAL
C                                       DERIVATIVES WERE USED, TO SIGNAL
C                                       THAT THEY MAY NEED UPDATING ON
C                                       SUBSEQUENT STEPS. THE ERROR TEST
C                                       IS MADE AND CONTROL PASSES TO
C                                       STATEMENT 190 IF IT FAILS.
  170 IF (MITER.NE.0) IWEVAL = -1
      NFE = NFE+M
      D = 0.
      DO 175 I=1,N
  175 D = D+(ERROR(I)/YMAX(I))**2
```

```
      IF (D.GT.E) GO TO 190
C                                        AFTER A SUCCESSFUL STEP, UPDATE THE
C                                          Y ARRAY. CONSIDER CHANGING H IF
C                                          IDOUB = 1. OTHERWISE DECREASE
C                                          IDOUB BY 1. IF IDOUB IS THEN 1 AND
C                                          NQ .LT. MAXDER, THEN ERROR IS
C                                          SAVED FOR USE IN A POSSIBLE ORDER
C                                          INCREASE ON THE NEXT STEP. IF A
C                                          CHANGE IN H IS CONSIDERED, AN
C                                          INCREASE OR DECREASE IN ORDER BY
C                                          ONE IS CONSIDERED ALSO. A CHANGE
C                                          IN H IS MADE ONLY IF IT IS BY A
C                                          FACTOR OF AT LEAST 1.1. IF NOT,
C                                          IDOUB IS SET TO 10 TO PREVENT
C                                          TESTING FOR THAT MANY STEPS.
      KFLAG = 0
      IREDO = 0
      NSTEP = NSTEP+1
      HUSED = H
      NQUSED = NQ
      DO 180 J=1,L
      DO 180 I=1,N
  180 Y(I,J) = Y(I,J)+EL(J)*ERROR(I)
      IF (IDOUB.EQ.1) GO TO 200
      IDOUB = IDOUB-1
      IF (IDOUB.GT.1) GO TO 290
      IF (L.EQ.LMAX) GO TO 290
      DO 185 I=1,N
  185 Y(I,LMAX) = ERROR(I)
      GO TO 290
C                                        THE ERROR TEST FAILED. KFLAG KEEPS
C                                          TRACK OF MULTIPLE FAILURES.
C                                          RESTORE T AND THE Y ARRAY TO THEIR
C                                          PREVIOUS VALUES, AND PREPARE TO
C                                          TRY THE STEP AGAIN. COMPUTE THE
C                                          OPTIMUM STEP SIZE FOR THIS OR ONE
C                                          LOWER ORDER.
  190 KFLAG = KFLAG-1
      T = TOLD
      DO 195 J1=1,NQ
      DO 195 J2=J1,NQ
         J = (NQ+J1)-J2
      DO 195 I=1,N
  195 Y(I,J) = Y(I,J)-Y(I,J+1)
      RMAX = 2.
      IF (ABS(H).LE.HMIN*1.00001) GO TO 270
      IF (KFLAG.LE.-3) GO TO 260
      IREDO = 2
      PR3 = 1.E+20
      GO TO 210
C                                        REGARDLESS OF THE SUCCESS OR FAILURE
C                                          OF THE STEP, FACTORS PR1, PR2, AND
C                                          PR3 ARE COMPUTED, BY WHICH H COULD
```

```
C                                       BE DIVIDED AT ORDER NQ - 1, ORDER
C                                       NQ, OR ORDER NQ + 1, RESPECTIVELY.
C                                       IN THE CASE OF FAILURE, PR3 =
C                                       1.E20 TO AVOID AN ORDER INCREASE.
C                                       THE SMALLEST OF THESE IS
C                                       DETERMINED AND THE NEW ORDER
C                                       CHOSEN ACCORDINGLY. IF THE ORDER
C                                       IS TO BE INCREASED, WE COMPUTE ONE
C                                       ADDITIONAL SCALED DERIVATIVE.
  200 PR3 = 1.E+20
      IF (L.EQ.LMAX) GO TO 210
      D1 = 0.
      DO 205 I=1,N
  205 D1 = D1+((ERROR(I)-Y(I,LMAX))/YMAX(I))**2
      ENQ3 = .5/(L+1)
      PR3 = ((D1/EUP)**ENQ3)*1.4+1.4E-6
  210 ENQ2 = .5/L
      PR2 = ((D/E)**ENQ2)*1.2+1.2E-6
      PR1 = 1.E+20
      IF (NQ.EQ.1) GO TO 220
      D = 0.
      DO 215 I=1,N
  215 D = D+(Y(I,L)/YMAX(I))**2
      ENQ1 = .5/NQ
      PR1 = ((D/EDN)**ENQ1)*1.3+1.3E-6
  220 IF (PR2.LE.PR3) GO TO 225
      IF (PR3.LT.PR1) GO TO 235
      GO TO 230
  225 IF (PR2.GT.PR1) GO TO 230
      NEWQ = NQ
      RH = 1./PR2
      GO TO 250
  230 NEWQ = NQ-1
      RH = 1./PR1
      IF (KFLAG.NE.0.AND.RH.GT.1.) RH = 1.
      GO TO 250
  235 NEWQ = L
      RH = 1./PR3
      IF (RH.LT.1.1) GO TO 245
      DO 240 I=1,N
  240 Y(I,NEWQ+1) = ERROR(I)*EL(L)/L
      GO TO 255
  245 IDOUB = 10
      GO TO 290
  250 IF ((KFLAG.EQ.0).AND.(RH.LT.1.1)) GO TO 245
C
C                                     IF THERE IS A CHANGE OF ORDER, RESET
C                                       NQ, L, AND THE COEFFICIENTS. IN
C                                       ANY CASE H IS RESET ACCORDING TO
C                                       RH AND THE Y ARRAY IS RESCALED.
C                                       THEN EXIT FROM 285 IF THE STEP WAS
C                                       OK, OR REDO THE STEP OTHERWISE.
      IF (NEWQ.EQ.NQ) GO TO 35
```

```
  255 NQ = NEWQ
      L = NQ+1
      IRET = 2
      GO TO 15
C                                     CONTROL REACHES THIS SECTION IF 3 OR
C                                       MORE FAILURES HAVE OCCURED. IT IS
C                                       ASSUMED THAT THE DERIVATIVES THAT
C                                       HAVE ACCUMULATED IN THE Y ARRAY
C                                       HAVE ERRORS OF THE WRONG ORDER.
C                                       HENCE THE FIRST DERIVATIVE IS
C                                       RECOMPUTED, AND THE ORDER IS SET
C                                       TO 1. THEN H IS REDUCED BY A
C                                       FACTOR OF 10, AND THE STEP IS
C                                       RETRIED. AFTER A TOTAL OF 7
C                                       FAILURES, AN EXIT IS TAKEN WITH
C                                       KFLAG = -2.
  260 IF (KFLAG.EQ.-7) GO TO 275
      RH = .1
      RH = AMAX1(HMIN/ABS(H),RH)
      H = H*RH
      CALL FCN (N,T,Y,SAVE1)
      NFE = NFE+1
      DO 265 I=1,N
  265 Y(I,2) = H*SAVE1(I)
      IWEVAL = MITER
      IDOUB = 10
      IF (NQ.EQ.1) GO TO 50
      NQ = 1
      L = 2
      IRET = 3
      GO TO 15
C                                     ALL RETURNS ARE MADE THROUGH THIS
C                                       SECTION. H IS SAVED IN HOLD TO
C                                       ALLOW THE CALLER TO CHANGE H ON
C                                       THE NEXT STEP.
  270 KFLAG = -1
      GO TO 290
  275 KFLAG = -2
      GO TO 290
  280 KFLAG = -3
      GO TO 290
  285 RMAX = 10.
  290 HOLD = H
      JSTART = NQ
      RETURN
      END
```

```
C    IMSL ROUTINE NAME    - LUDATF
C
C-----------------------------------------------------------------------
C
C    COMPUTER             - BGH/SINGLE
C
C    LATEST REVISION      - JANUARY 1, 1978
C
C    PURPOSE              - L-U DECOMPOSITION BY THE CROUT ALGORITHM
C                           WITH OPTIONAL ACCURACY TEST.
C
C    USAGE                - CALL LUDATF (A,LU,N,IA,IDGT,D1,D2,IPVT,
C                           EQUIL,WA,IER)
C
C    ARGUMENTS    A       - INPUT MATRIX OF DIMENSION N BY N CONTAINING
C                           THE MATRIX TO BE DECOMPOSED.
C                 LU      - REAL OUTPUT MATRIX OF DIMENSION N BY N
C                           CONTAINING THE L-U DECOMPOSITION OF A
C                           ROWWISE PERMUTATION OF THE INPUT MATRIX.
C                           FOR A DESCRIPTION OF THE FORMAT OF LU, SEE
C                           EXAMPLE.
C                 N       - INPUT SCALAR CONTAINING THE ORDER OF THE
C                           MATRIX A.
C                 IA      - INPUT SCALAR CONTAINING THE ROW DIMENSION OF
C                           MATRICES A AND LU EXACTLY AS SPECIFIED IN
C                           THE CALLING PROGRAM.
C                 IDGT    - INPUT OPTION.
C                           IF IDGT IS GREATER THAN ZERO, THE NON-ZERO
C                           ELEMENTS OF A ARE ASSUMED TO BE CORRECT TO
C                           IDGT DECIMAL PLACES.  LUDATF PERFORMS AN
C                           ACCURACY TEST TO DETERMINE IF THE COMPUTED
C                           DECOMPOSITION IS THE EXACT DECOMPOSITION
C                           OF A MATRIX WHICH DIFFERS FROM THE GIVEN
C                           ONE BY LESS THAN ITS UNCERTAINTY.
C                         IF IDGT IS EQUAL TO ZERO, THE ACCURACY TEST
C                           IS BYPASSED.
C                 D1      - OUTPUT SCALAR CONTAINING ONE OF THE TWO
C                           COMPONENTS OF THE DETERMINANT. SEE
C                           DESCRIPTION OF PARAMETER D2, BELOW.
C                 D2      - OUTPUT SCALAR CONTAINING ONE OF THE
C                           TWO COMPONENTS OF THE DETERMINANT. THE
C                           DETERMINANT MAY BE EVALUATED AS (D1)(2**D2).
C                 IPVT    - OUTPUT VECTOR OF LENGTH N CONTAINING THE
C                           PERMUTATION INDICES. SEE DOCUMENT
C                           (ALGORITHM).
C                 EQUIL   - OUTPUT VECTOR OF LENGTH N CONTAINING
C                           RECIPROCALS OF THE ABSOLUTE VALUES OF
C                           THE LARGEST (IN ABSOLUTE VALUE) ELEMENT
C                           IN EACH ROW.
C                 WA      - ACCURACY TEST PARAMETER, OUTPUT ONLY IF
C                           IDGT IS GREATER THAN ZERO.
C                           SEE ELEMENT DOCUMENTATION FOR DETAILS.
C                 IER     - ERROR PARAMETER. (OUTPUT)
```

```
C                          TERMINAL ERROR
C                            IER = 129 INDICATES THAT MATRIX A IS
C                              ALGORITHMICALLY SINGULAR. (SEE THE
C                              CHAPTER L PRELUDE).
C                          WARNING ERROR
C                            IER = 34 INDICATES THAT THE ACCURACY TEST
C                              FAILED.  THE COMPUTED SOLUTION MAY BE IN
C                              ERROR BY MORE THAN CAN BE ACCOUNTED FOR
C                              BY THE UNCERTAINTY OF THE DATA.  THIS
C                              WARNING CAN BE PRODUCED ONLY IF IDGT IS
C                              GREATER THAN 0 ON INPUT.  SEE CHAPTER L
C                              PRELUDE FOR FURTHER DISCUSSION.
C
C    PRECISION/HARDWARE   - SINGLE AND DOUBLE/H32
C                         - SINGLE/H36,H48,H60
C
C    REQD. IMSL ROUTINES  - UERTST,UGETIO
C
C    NOTATION             - INFORMATION ON SPECIAL NOTATION AND
C                             CONVENTIONS IS AVAILABLE IN THE MANUAL
C                             INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
C
C    REMARKS      A TEST FOR SINGULARITY IS MADE AT TWO LEVELS:
C                 1.  A ROW OF THE ORIGINAL MATRIX A IS NULL.
C                 2.  A COLUMN BECOMES NULL IN THE FACTORIZATION PROCESS.
C
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C
C    WARRANTY             - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN
C                             APPLIED TO THIS CODE. NO OTHER WARRANTY,
C                             EXPRESSED OR IMPLIED, IS APPLICABLE.
C
C
C=====================================================================
      SUBROUTINE LUDATF (A,LU,N,IA,IDGT,D1,D2,IPVT,EQUIL,WA,IER)
C=====================================================================
      DIMENSION          A(IA,1),LU(IA,1),IPVT(1),EQUIL(1)
      REAL               LU
      DATA               ZERO,ONE,FOUR,SIXTN,SIXTH/0.0,1.,4.,16.,.0625/
C---------------------------------------------------------------------
C                                  INITIALIZATION
      IER = 0
      RN = N
      WREL = ZERO
      D1 = ONE
      D2 = ZERO
      BIGA = ZERO
      DO 10 I=1,N
         BIG = ZERO
         DO 5 J=1,N
            P = A(I,J)
            LU(I,J) = P
            P = ABS(P)
```

```
            IF (P .GT. BIG) BIG = P
    5     CONTINUE
          IF (BIG .GT. BIGA) BIGA = BIG
          IF (BIG .EQ. ZERO) GO TO 110
          EQUIL(I) = ONE/BIG
   10   CONTINUE
        DO 105 J=1,N
          JM1 = J-1
          IF (JM1 .LT. 1) GO TO 40
C                                       COMPUTE U(I,J), I=1,...,J-1
          DO 35 I=1,JM1
            SUM = LU(I,J)
            IM1 = I-1
            IF (IDGT .EQ. 0) GO TO 25
C                                       WITH ACCURACY TEST
            AI = ABS(SUM)
            WI = ZERO
            IF (IM1 .LT. 1) GO TO 20
            DO 15 K=1,IM1
              T = LU(I,K)*LU(K,J)
              SUM = SUM-T
              WI = WI+ABS(T)
   15       CONTINUE
            LU(I,J) = SUM
   20       WI = WI+ABS(SUM)
            IF (AI .EQ. ZERO) AI = BIGA
            TEST = WI/AI
            IF (TEST .GT. WREL) WREL = TEST
            GO TO 35
C                                       WITHOUT ACCURACY
   25       IF (IM1 .LT. 1) GO TO 35
            DO 30 K=1,IM1
              SUM = SUM-LU(I,K)*LU(K,J)
   30       CONTINUE
            LU(I,J) = SUM
   35     CONTINUE
   40     P = ZERO
C                                       COMPUTE U(J,J) AND L(I,J), I=J+1,...,
          DO 70 I=J,N
            SUM = LU(I,J)
            IF (IDGT .EQ. 0) GO TO 55
C                                       WITH ACCURACY TEST
            AI = ABS(SUM)
            WI = ZERO
            IF (JM1 .LT. 1) GO TO 50
            DO 45 K=1,JM1
              T = LU(I,K)*LU(K,J)
              SUM = SUM-T
              WI = WI+ABS(T)
   45       CONTINUE
            LU(I,J) = SUM
   50       WI = WI+ABS(SUM)
            IF (AI .EQ. ZERO) AI = BIGA
```

```
            TEST = WI/AI
            IF (TEST .GT. WREL) WREL = TEST
            GO TO 65
C                                   WITHOUT ACCURACY TEST
   55       IF (JM1 .LT. 1) GO TO 65
            DO 60 K=1,JM1
               SUM = SUM-LU(I,K)*LU(K,J)
   60       CONTINUE
            LU(I,J) = SUM
   65       Q = EQUIL(I)*ABS(SUM)
            IF (P .GE. Q) GO TO 70
            P = Q
            IMAX = I
   70    CONTINUE
C                                   TEST FOR ALGORITHMIC SINGULARITY
         IF (RN+P .EQ. RN) GO TO 110
         IF (J .EQ. IMAX) GO TO 80
C                                   INTERCHANGE ROWS J AND IMAX
         D1 = -D1
         DO 75 K=1,N
            P = LU(IMAX,K)
            LU(IMAX,K) = LU(J,K)
            LU(J,K) = P
   75    CONTINUE
         EQUIL(IMAX) = EQUIL(J)
   80    IPVT(J) = IMAX
         D1 = D1*LU(J,J)
   85    IF (ABS(D1) .LE. ONE) GO TO 90
         D1 = D1*SIXTH
         D2 = D2+FOUR
         GO TO 85
   90    IF (ABS(D1) .GE. SIXTH) GO TO 95
         D1 = D1*SIXTN
         D2 = D2-FOUR
         GO TO 90
   95    CONTINUE
         JP1 = J+1
         IF (JP1 .GT. N) GO TO 105
C                                   DIVIDE BY PIVOT ELEMENT U(J,J)
         P = LU(J,J)
         DO 100 I=JP1,N
            LU(I,J) = LU(I,J)/P
  100    CONTINUE
  105 CONTINUE
C                                   PERFORM ACCURACY TEST
      IF (IDGT .EQ. 0) GO TO 9005
      P = 3*N+3
      WA = P*WREL
      IF (WA+10.0**(-IDGT) .NE. WA) GO TO 9005
      IER = 34
      GO TO 9000
C                                   ALGORITHMIC SINGULARITY
  110 IER = 129
```

```
      D1 = ZERO
      D2 = ZERO
 9000 CONTINUE
C                                          PRINT ERROR
      CALL UERTST(IER,6HLUDATF)
 9005 RETURN
      END
```

```
C    IMSL ROUTINE NAME   - LUELMF
C
C-----------------------------------------------------------------------
C
C    COMPUTER            - BGH/SINGLE
C
C    LATEST REVISION     - JANUARY 1, 1978
C
C    PURPOSE             - ELIMINATION PART OF SOLUTION OF AX=B
C                            (FULL STORAGE MODE)
C
C    USAGE               - CALL LUELMF (A,B,IPVT,N,IA,X)
C
C    ARGUMENTS     A     - A = LU (THE RESULT COMPUTED IN THE IMSL
C                            ROUTINE LUDATF) WHERE L IS A LOWER
C                            TRIANGULAR MATRIX WITH ONES ON THE MAIN
C                            DIAGONAL. U IS UPPER TRIANGULAR. L AND U
C                            ARE STORED AS A SINGLE MATRIX A AND THE
C                            UNIT DIAGONAL OF L IS NOT STORED. (INPUT)
C                   B     - B IS A VECTOR OF LENGTH N ON THE RIGHT HAND
C                            SIDE OF THE EQUATION AX=B. (INPUT)
C                   IPVT  - THE PERMUTATION MATRIX RETURNED FROM THE
C                            IMSL ROUTINE LUDATF, STORED AS AN N LENGTH
C                            VECTOR. (INPUT)
C                   N     - ORDER OF A AND NUMBER OF ROWS IN B. (INPUT)
C                   IA    - ROW DIMENSION OF A EXACTLY AS SPECIFIED IN
C                            THE DIMENSION STATEMENT IN THE CALLING
C                            PROGRAM. (INPUT)
C                   X     - THE RESULT X. (OUTPUT)
C
C    PRECISION/HARDWARE  - SINGLE AND DOUBLE/H32
C                        - SINGLE/H36,H48,H60
C
C    REQD. IMSL ROUTINES - NONE REQUIRED
C
C    NOTATION            - INFORMATION ON SPECIAL NOTATION AND
C                            CONVENTIONS IS AVAILABLE IN THE MANUAL
C                            INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
C
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C                            EXPRESSED OR IMPLIED, IS APPLICABLE.
C
C
C=======================================================================
      SUBROUTINE LUELMF (A,B,IPVT,N,IA,X)
C=======================================================================
      DIMENSION          A(IA,1),B(1),IPVT(1),X(1)
C-----------------------------------------------------------------------
C                                  SOLVE LY = B FOR Y
      DO 5 I=1,N
```

```
    5 X(I) = B(I)
      IW = 0
      DO 20 I=1,N
         IP = IPVT(I)
         SUM = X(IP)
         X(IP) = X(I)
         IF (IW .EQ. 0) GO TO 15
         IM1 = I-1
         DO 10 J=IW,IM1
            SUM = SUM-A(I,J)*X(J)
   10    CONTINUE
         GO TO 20
   15    IF (SUM .NE. 0.) IW = I
   20 X(I) = SUM
C                                        SOLVE UX = Y FOR X
      DO 30 IB=1,N
         I = N+1-IB
         IP1 = I+1
         SUM = X(I)
         IF (IP1 .GT. N) GO TO 30
         DO 25 J=IP1,N
            SUM = SUM-A(I,J)*X(J)
   25   CONTINUE
   30 X(I) = SUM/A(I,I)
      RETURN
      END
```

```
C    IMSL ROUTINE NAME    - UERTST
C
C-----------------------------------------------------------------------
C
C    COMPUTER             - BGH/SINGLE
C
C    LATEST REVISION      - JANUARY 1, 1978
C
C    PURPOSE              - PRINT A MESSAGE REFLECTING AN ERROR CONDITION
C
C    USAGE                - CALL UERTST (IER,NAME)
C
C    ARGUMENTS    IER     - ERROR PARAMETER. (INPUT)
C                             IER = I+J WHERE
C                               I = 128 IMPLIES TERMINAL ERROR,
C                               I =  64 IMPLIES WARNING WITH FIX, AND
C                               I =  32 IMPLIES WARNING.
C                               J = ERROR CODE RELEVANT TO CALLING
C                                   ROUTINE.
C                 NAME    - A SIX CHARACTER LITERAL STRING GIVING THE
C                             NAME OF THE CALLING ROUTINE. (INPUT)
C
C    PRECISION/HARDWARE   - SINGLE/ALL
C
C    REQD. IMSL ROUTINES  - UGETIO
C
C    NOTATION             - INFORMATION ON SPECIAL NOTATION AND
C                             CONVENTIONS IS AVAILABLE IN THE MANUAL
C                             INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
C
C    REMARKS      THE ERROR MESSAGE PRODUCED BY UERTST IS WRITTEN
C                 ONTO THE STANDARD OUTPUT UNIT. THE OUTPUT UNIT
C                 NUMBER CAN BE DETERMINED BY CALLING UGETIO AS
C                 FOLLOWS..   CALL UGETIO(1,NIN,NOUT).
C                 THE OUTPUT UNIT NUMBER CAN BE CHANGED BY CALLING
C                 UGETIO AS FOLLOWS..
C                                 NIN = 0
C                                 NOUT = NEW OUTPUT UNIT NUMBER
C                                 CALL UGETIO(3,NIN,NOUT)
C                 SEE THE UGETIO DOCUMENT FOR MORE DETAILS.
C
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C                             EXPRESSED OR IMPLIED, IS APPLICABLE.
C
C
C=======================================================================
      SUBROUTINE UERTST (IER,NAME)
C=======================================================================
      INTEGER              IER,NAME
C                                  SPECIFICATIONS FOR LOCAL VARIABLES
```

```
      INTEGER             NAMSET,NAMEQ
      DATA                NAMSET/6HUERSET/
      DATA                NAMEQ/6H      /
C-----------------------------------------------------------------------
      DATA                LEVEL/4/,IEQDF/0/,IEQ/1H=/
      IF (IER.GT.999) GO TO 25
      IF (IER.LT.-32) GO TO 55
      IF (IER.LE.128) GO TO 5
      IF (LEVEL.LT.1) GO TO 30
C                                 PRINT TERMINAL MESSAGE
      CALL UGETIO(1,NIN,IOUNIT)
      IF (IEQDF.EQ.1) WRITE(IOUNIT,35) IER,NAMEQ,IEQ,NAME
      IF (IEQDF.EQ.0) WRITE(IOUNIT,35) IER,NAME
      GO TO 30
    5 IF (IER.LE.64) GO TO 10
      IF (LEVEL.LT.2) GO TO 30
C                                 PRINT WARNING WITH FIX MESSAGE
      CALL UGETIO(1,NIN,IOUNIT)
      IF (IEQDF.EQ.1) WRITE(IOUNIT,40) IER,NAMEQ,IEQ,NAME
      IF (IEQDF.EQ.0) WRITE(IOUNIT,40) IER,NAME
      GO TO 30
   10 IF (IER.LE.32) GO TO 15
C                                 PRINT WARNING MESSAGE
      IF (LEVEL.LT.3) GO TO 30
      CALL UGETIO(1,NIN,IOUNIT)
      IF (IEQDF.EQ.1) WRITE(IOUNIT,45) IER,NAMEQ,IEQ,NAME
      IF (IEQDF.EQ.0) WRITE(IOUNIT,45) IER,NAME
      GO TO 30
   15 CONTINUE
C                                 CHECK FOR UERSET CALL
      IF (NAME.NE.NAMSET) GO TO 25
      LEVOLD = LEVEL
      LEVEL = IER
      IER = LEVOLD
      IF (LEVEL.LT.0) LEVEL = 4
      IF (LEVEL.GT.4) LEVEL = 4
      GO TO 30
   25 CONTINUE
      IF (LEVEL.LT.4) GO TO 30
C                                 PRINT NON-DEFINED MESSAGE
      CALL UGETIO(1,NIN,IOUNIT)
      IF (IEQDF.EQ.1) WRITE(IOUNIT,50) IER,NAMEQ,IEQ,NAME
      IF (IEQDF.EQ.0) WRITE(IOUNIT,50) IER,NAME
   30 IEQDF = 0
      RETURN
   35 FORMAT(19H *** TERMINAL ERROR,10X,7H(IER = ,I3,
     1        20H) FROM IMSL ROUTINE ,A6,A1,A6)
   40 FORMAT(36H *** WARNING WITH FIX ERROR  (IER = ,I3,
     1        20H) FROM IMSL ROUTINE ,A6,A1,A6)
   45 FORMAT(18H *** WARNING ERROR,11X,7H(IER = ,I3,
     1        20H) FROM IMSL ROUTINE ,A6,A1,A6)
   50 FORMAT(20H *** UNDEFINED ERROR,9X,7H(IER = ,I5,
     1        20H) FROM IMSL ROUTINE ,A6,A1,A6)
```

```
                SAVE P FOR P = R CASE
                  P IS THE PAGE NAME
                  R IS THE ROUTINE NAME

55 IEQDF = 1
   NAMEQ = NAME
65 RETURN
   END
```

```
C    IMSL ROUTINE NAME   - UGETIO
C
C-----------------------------------------------------------------------
C
C    COMPUTER            - BGH/SINGLE
C
C    LATEST REVISION     - JANUARY 1, 1978
C
C    PURPOSE             - TO RETRIEVE CURRENT VALUES AND TO SET NEW
C                          VALUES FOR INPUT AND OUTPUT UNIT
C                          IDENTIFIERS.
C
C    USAGE               - CALL UGETIO(IOPT,NIN,NOUT)
C
C    ARGUMENTS    IOPT   - OPTION PARAMETER. (INPUT)
C                          IF IOPT=1, THE CURRENT INPUT AND OUTPUT
C                          UNIT IDENTIFIER VALUES ARE RETURNED IN NIN
C                          AND NOUT, RESPECTIVELY.
C                          IF IOPT=2 (3) THE INTERNAL VALUE OF
C                          NIN (NOUT) IS RESET FOR SUBSEQUENT USE.
C                 NIN    - INPUT UNIT IDENTIFIER.
C                          OUTPUT IF IOPT=1, INPUT IF IOPT=2.
C                 NOUT   - OUTPUT UNIT IDENTIFIER.
C                          OUTPUT IF IOPT=1, INPUT IF IOPT=3.
C
C    PRECISION/HARDWARE  - SINGLE/ALL
C
C    REQD. IMSL ROUTINES - NONE REQUIRED
C
C    NOTATION            - INFORMATION ON SPECIAL NOTATION AND
C                          CONVENTIONS IS AVAILABLE IN THE MANUAL
C                          INTRODUCTION OR THROUGH IMSL ROUTINE UHELP
C
C    REMARKS      EACH IMSL ROUTINE THAT PERFORMS INPUT AND/OR OUTPUT
C                 OPERATIONS CALLS UGETIO TO OBTAIN THE CURRENT UNIT
C                 IDENTIFIER VALUES. IF UGETIO IS CALLED WITH IOPT=2 OR 3
C                 NEW UNIT IDENTIFIER VALUES ARE ESTABLISHED. SUBSEQUENT
C                 INPUT/OUTPUT IS PERFORMED ON THE NEW UNITS.
C
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C
C    WARRANTY            - IMSL WARRANTS ONLY THAT IMSL TESTING HAS BEEN
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C                          EXPRESSED OR IMPLIED, IS APPLICABLE.
C
C
C-----------------------------------------------------------------------
      SUBROUTINE UGETIO(IOPT,NIN,NOUT)
C-----------------------------------------------------------------------
      INTEGER             IOPT,NIN,NOUT
C                                 SPECIFICATIONS FOR LOCAL VARIABLES
      INTEGER             NIND,NOUTD
      DATA                NIND/5/,NOUTD/6/
```

```
      IF (IOPT.EQ.3) GO TO 10
      IF (IOPT.EQ.2) GO TO 5
      IF (IOPT.NE.1) GO TO 9005
      NIN = NINO
      NOUT = NOUTO
      GO TO 9005
    5 NIN = NINO
      GO TO 9005
   10 NOUTO = NOUT
 9005 RETURN
      END
```

THIS IS THE INPUT DATA FILE INPUT.DAT.
REFER TO THE FOLLOWING PAGE FOR A DESCRIPTION OF THIS DATA.

```
0.022     480.     298.
0.025    0.038    0.089    0.2
0.1982   0.1500   0.7990   0.0028
0.0028   0.4922   0.0606   0.0000   0.4444
0.020     348.       1.
0.0      0.23     0.77
0.03
 298.
...0      1.02       1.0
1         3
2         3
4         3
1.0E-6
 100      10
0.001    0.00001 0.001
 373.
```

The data in the file INPUT.DAT are as follows:

wood feedrate (wet basis - kg/s)
wood particle density (wet basis - kg/m3)
packed bed density (wet basis - kg/m3)

half-width of the wood particle (m)
breadth of the wood particle (m)
height of the wood particle (m)

fixed carbon fraction from proximate analysis (dry basis)
fractional moisture content of wood (wet basis)
volatile fraction from proximate analysis (dry basis)
ash fraction from proximate analysis (dry basis)

ash fraction from ultimate analysis (dry basis)
carbon fraction from ultimate analysis (dry basis)
hydrogen fraction from ultimate analysis (dry basis)
nitrogen fraction from ultimate analysis (dry basis)
oxygen fraction from ultimate analysis (dry basis)

feedrate of air (wet basis - kg/s)
temperature of air feed (K)
pressure of air feed (atm)

water mass fraction in air feed
oxygen mass fraction in air feed
nitrogen mass fraction in air feed

half-width of the air distribution region (m)

ambient temperature (K)

height of the packed bed (m)
location of the tuyeres (measured from the top - m)
pressure in the gasifier (atm)

basic method indicator for drying zone
iteration method indicator for drying zone

basic method indicator for pyrolysis zone
iteration method indicator for pyrolysis zone

basic method indicator for combustion (and subsequent) zones
iteration method indicator for combustion (and subsequent) zones

error bound for the numerical solution in DGEAR

number of compartments in gasifier for the integration

maximum number of complete profile iterations

initial step size in drying zone (DGEAR)
initial step size in pyrolysis zone (DGEAR)
initial step size in combustion (and subsequent) zones (DGEAR)

initial estimate of the temperature at the top of the bed

Appendix A.6.5 : Instructions for Executing the Simulation Program

The simulation program QUGAS2 (version 83-09) is written in FORTRAN. It was developed on a PDP 11 V23 minicomputer with two dual density floppy disk drives. Some text editing is required to execute the program. The following instructions are for a PDP 11 V23 with a Q'TEXT text editing package.

1. In command mode, FEtch INPUT.DAT file. Edit this file to incorporate the specific operating instructions which are to be examined. (The data format in the current file should be adhered to. Refer to Appendix A.3 for details about the data contained in this file.)

2. After all required changes have been made press the keys CTRL and C simultaneously. Type OVerwrite INPUT.DAT and RETURN. The new data file will replace the previous file.

3. The program is now ready to run. Type GOodbye and RETURN to enter the system mode. Check that the printer is ONLINE. Then type RUN QUGAS2. Version 83-09 runs in a batch mode.

POOR

QUALITY

ORIGINAL